Final Technical Report

Transport Modeling of Hydrogen in Metals for Application to Hydrogen Assisted Cracking of Metals

by

Dr. James P. Thomas (PI) and Mr. Charles E. Chopin

for the

Office of Naval Research
Grant Number: N00014-93-1-0845

DTIC
ELECTE
OCT 1 6 1995
F

Department of Aerospace and Mechanical Engineering

University of Notre Dame
Notre Dame, Indiana 46556

DISTRIBUTION STATEMENT A
Approved for public release;
Distribution Unlimited

19951012 037

TR: 001-4/95

Final Technical Report

Transport Modeling of Hydrogen in Metals for Application to Hydrogen Assisted Cracking of Metals

by

Dr. James P. Thomas (PI) and Mr. Charles E. Chopin

for the

Office of Naval Research

Grant Number: N00014-93-1-0845

DTIC
ELECTE
OCT 1 6 1995
F

Accesion For
NTIS CRA&I
DTIC TAB
Unannounced
Justification
By per ltr
Distribution /
Availability Codes
Dist | Avail and / or Special
A-1

DISTRIBUTION STATEMENT A
Approved for public release;
Distribution Unlimited

TR: 001-4/95

Final Technical Report

Transport Modeling of Hydrogen in Metals for Application to Hydrogen Assisted Cracking of Metals

submitted by:

Dr. James P. Thomas[‡] and Mr. Charles E. Chopin[†]
University of Notre Dame
Department of Aerospace and Mechanical Engineering
Notre Dame, Indiana 46556-5637

April 4, 1995

submitted to:

Dr. A. John Sedriks, Code 3312
Office of Naval Research
Ballston Tower One
800 North Quincy Street
Arlington, Virginia 22217-5660

Grant Number: N00014-93-1-0845
September 1, 1993 to December 31, 1994

[‡] Principal Investigator, Assistant Professor.
[†] Graduate Research Assistant

TABLE OF CONTENTS

ONR Contract Information ..... *iii*
Executive Summary ..... *iv*
Final Report *1*
Introduction *1*
Theoretical Modeling *3*
Balance Equations *3*
Trapping Analysis *4*
Constitutive Equations *4*
Governing Equations *6*
Finite Element Modeling *6*
Programming Simplifications *7*
Formulation of the Finite Element Matrix Equations *8*
Interpolation Functions for the Concentration and Displacement *8*
Isoparametric Interpolation Functions *10*
Gauss-Legendre Numerical Integration *11*
Finite Element Equations *12*
Non-Linear Solutions via Newton-Raphson *13*
Re-Ordering the Degrees of Freedom *14*
ABAQUS User Element Subroutines *15*
Modeling Applications *16*
Results *17*
Case 1 and 2 Problems *17*
Case 3 Problems *21*
Discussion *24*
Summary and Future Research *26*
Acknowledgments *27*
References *28*

Appendix A: Analytical Solutions via Maple *A-1*
Appendix B: User Element Subroutine *B-1*
Appendix C: Sample Input Deck *C-1*
Appendix D: Sample Output *D-1*
Appendix E: Conference Paper *E-1*
Appendix F: Summary of Publications/Reports/Presentations During Grant Period *F-1*

ONR CONTRACT INFORMATION

Contract Title: "Transport Modeling of Hydrogen in Metals
For Application to Hydrogen Assisted Cracking"

Performing Organization: University of Notre Dame

Principal Investigator: Dr. James P. Thomas

Contract Number: N00014-93-1-0845

R & T Project Number: cor5247---01

ONR Scientific Officer: Dr. A. John Sedriks, Code 3312

EXECUTIVE SUMMARY

The focus of this research was on the development of a finite element code for solute transport and trapping in linear elastic mixtures for use in modeling the hydrogen transport process in metals undergoing hydrogen assisted cracking. Specific objectives included:

1.) Completion of the development of a solute transport and trapping model with coupling between the concentration, deformation, and thermal field variables and trapping at reversible and irreversible trap sites.

2.) Implementation of the above theory in a finite element code.

3.) Calculation of the crack tip deformations and chemical state variables for some high strength steels under a variety of loading, environment, and material conditions.

A solute transport model has been developed for linear elastic mixtures with coupling between the deformation, concentration, and thermal variables and trapping at reversible and irreversible trap sites. A journal publication describing this model is in preparation[1].

Work on a 2-D finite element implementation and its application to the modeling of hydrogen transport in a cracking metal is ongoing. A 1-D code has been developed and tested on a variety of problems with known analytical solutions. The "code" consists of a Fortran "user element" subroutine for use with the ABAQUS[2] finite element program. Documentation of the 1-D user element subroutine is contained within this report.

Work on objective **3.)** could not be started without a 2-D version of the finite element code. The 1-D code was used to model a variety of hydrogen transport problems with the objective of learning more about the fully coupled transport theory. We were able to "invent" a problem with a square-root singular stress ($\sigma_x \sim 1/\sqrt{x}$). This problem was used to gain preliminary insight into the hydrogen distribution problem in planar crack geometries. The problem consisted of subjecting a 4340 steel rod ($10\ cm \times 1\ cm^2$) to a singular body force ($\sim 1/x^{3/2}$) resulting in the square root singular stress. The steady-state hydrogen concentrations and deformations were determined using the fully coupled theory, developed in this work, and classical stress assisted diffusion (SAD) theory.

The fully coupled predictions showed slightly higher hydrogen concentrations, a more severe singularity in the concentration, larger axial and dilatational strains, and larger axial displacements, all of which depended on the extent of hydrogen trapping. The mathematical solution for the concentration became multi-valued as the singularity was approached. It was shown that this "non-physical" result would be eliminated if the product of the density, the molar volume of hydrogen in the mixture, and the bulk modulus decrease linearly or better with increasing hydrogen concentration. These findings are documented in the report and in a conference paper included as Appendix E.

Development of a 2-D user element subroutine is ongoing. The 2-D code will initially be limited to simple linear elastic mixture behavior and equilibrium trapping. Extensions of the model to include non-equilibrium trapping effects and plastic crack tip deformations are planned. An effort is also being made to interface the ABAQUS code with our user element routines to the Patran[3] Solid Geometry Modeling program for more convenient meshing of complex 2-D geometries and for displaying the finite element results.

---

[1] J. P. Thomas and P. Matic, "Solute Transport Modeling in Elastic Solids", *Int. J. Engnr. Sci.*, in preparation.

[2] ABAQUS is a finite element code supported by HKS, Inc., Pawtucket, RI.

[3] Patran is a solid geometry modeling program supported by PDA Engineering, Costa Mesa, CA.

TRANSPORT MODELING OF HYDROGEN IN METALS FOR APPLICATION TO HYDROGEN ASSISTED CRACKING

INTRODUCTION

Two fundamental questions naturally arise in modeling the influence of hydrogen on the crack growth rate of metals. Namely, how does hydrogen "enhance" the crack growth rate (CGR); and what is the relationship between the hydrogen distribution within the material and the corresponding "enhancement" in the CGR? Quantitative knowledge of the crack tip hydrogen distribution under service or laboratory test conditions is requisite to addressing these questions and will require: **a)** a hydrogen transport model that incorporates trapping and deformation-concentration coupling effects (governing equations); **b)** knowledge of the time dependent, non-uniform hydrogen distribution along the crack walls (boundary conditions); and **c)** a mathematical solution technique for the resulting system of non-linear equations.

Stress-assisted diffusion (SAD) theory [1,2] is commonly used to model hydrogen transport in cracking metals systems. This theory extends classical diffusion by adding a hydrostatic stress gradient term as a driving force for diffusive transport. Equilibrium trapping effects are included through the use of an effective diffusion coefficient.

The influence of hydrogen on the material deformation state is assumed to be negligible, and this uncouples the deformation equations from the concentration variable. Hydrostatic stresses determined from solutions to standard elasticity or plasticity problems are used with the SAD equation to solve for the resulting concentration. The steady-state hydrogen distribution for Mode I cracks in linear elastic materials with uniform hydrogen concentration along the boundaries is given by [2]:

$$c = c_0 exp\left(constant \times \frac{K}{\sqrt{r}} cos\frac{\theta}{2} \right)$$

where c_0 is the boundary concentration, K is the stress intensity factor, and r and θ are polar coordinates centered at the crack tip. Note that $c \rightarrow \infty$ as $r \rightarrow 0$ (the crack tip).

Transient and steady-state hydrogen distributions for a plastically deforming crack in iron have been obtained by Sofronis & McMeeking [3] using finite element methods. Their results show large, but finite, concentrations at the crack tip region, primarily in traps near the crack surface. They conclude that the crack tip hydrogen distribution is primarily determined by the creation of dislocation traps via plastic straining at the crack tip.

Damage models that attempt to link the crack tip hydrogen distribution to the fracture process have been reviewed in [4-6]. Applications to service cracking problems have met with some success, but the lack of information on the crack wall hydrogen distributions under service or laboratory conditions has limited the usefulness of these models.

The task of specifying the crack wall hydrogen distribution is difficult because of the complex nature of the interacting chemical, mechanical, and metallurgical processes operative during hydrogen assisted cracking of metals (Fig.1). In aqueous systems, the hydrogen production process is driven by the rapid and irreversible evolution of the chemically unstable "bare" surface at the crack tip to a more stable equilibrium "filmed" state. An electron flow is induced between the bare and filmed crack flank surfaces; net

anodic (dissolution/filming) reactions take place on the bare surface and net cathodic (hydrogen reduction) reactions take place on the filmed surfaces.

Adsorbed hydrogen, H_{ads}, can be produced on both the bare and filmed crack surfaces by: **(1)** the reduction of hydrogen ions in acidic environments; or **(2)** by the reduction of water in alkaline environments. The MH_{ads} species are then free to be absorbed by the transition reaction **(a)**; or combine to form H_2 gas via: recombination **(b1)**; or electrochemical desorption **(b2)**. Reactions **(a)**, **(b1)**, and **(b2)** occur in parallel, but one of the two **(b1)** or **(b2)** reactions is usually dominant (Fig.2).

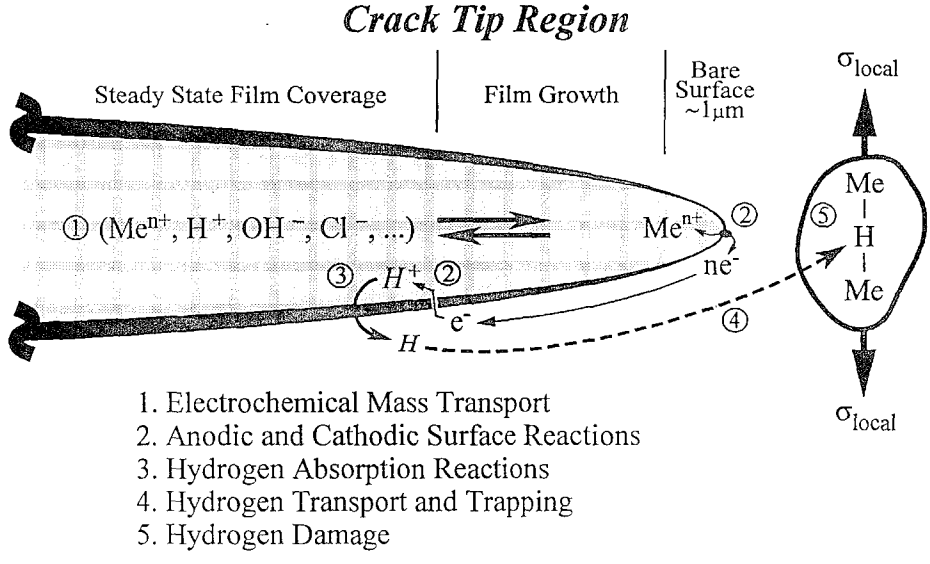


Figure 1: Schematic of the processes responsible for hydrogen assisted crack growth.

(1) ***Acidic:***	$M + H^+ + e^- \Leftrightarrow MH_{ads}$
(2) ***Alkaline:***	$M + H_2O + e^- \Leftrightarrow MH_{ads} + OH^-$

(a) ***Adsorption-Absorption:***	$MH_{ads} \Leftrightarrow MH_{abs}$
(b1) ***Recombination:***	$MH_{ads} + MH_{ads} \Leftrightarrow H_2 + 2M$
(b2) ***EC Desorption:***	$MH_{ads} + H^+ + e^- \Leftrightarrow H_2 + M$

Figure 2: Summary of the hydrogen producing reactions.

The distribution of MH_{abs} along the crack surface is governed by the surface coverage of MH_{ads} and the kinetics of reaction **(a)** acting in parallel with reaction **(b1)** or **(b2)**. These factors are influenced, in turn, by: the electrochemical environment at the crack tip region (e.g., the potential, pH, species concentrations, dissolved O_2, etc.); the kinetics of the bare and filmed surface reactions; and the rate of transport of H_{abs} from the crack surface into the material.

Iyer and Pickering [7] have reviewed and modeled the kinetics of hydrogen evolution and entry in stress free metallic systems with homogeneous electrochemical conditions at the metal surface. Their model is used to quantify the rate constants associated with reactions **(1)** or **(2)** and **(a)** and **(b1)** or **(b2)** via analysis of experimental permeation data. Turnbull [8] has reviewed electrochemical conditions in cracks with particular emphasis on corrosion fatigue cracks of structural steels in sea water. Similarly, Beck [9] and Newman [10] have examined experimental techniques for characterizing bare (and filmed) surface reaction kinetics. The above models, data, and techniques, plus information concerning the rate controlling process during crack growth, will have to be used in an analysis of the mass transport process within the crack to develop realistic predictions of the MH_{abs} distribution.

We begin with a description of fully coupled transport and trapping theory. The use of the ABAQUS finite element "User Element" subroutines for solving 1-D problems is then outlined in full detail. This is followed by a description of three 1-D rod problems that have been studied. The results of these studies are reported next, followed by a discussion. And finally, some conclusions are drawn, and suggestions are made for further research.

THEORETICAL MODELING

This section begins with a brief description of the theory adopted for modeling coupled diffusion/trapping processes. Derivation of the finite element equations using the method of weighted residuals is described, followed by a description of analytical and finite element solutions to three simple steady-state hydrogen transport problems. While the motivation for this work is the modeling of hydrogen transport in cracking metal systems, the formulation presented here is generalized to generic solute-solid mixtures.

Three solute species are modeled in the analysis:

$S_L \equiv$ interstitial or lattice species
$S_R \equiv$ weak or moderately (reversibly) trapped species
$S_I \equiv$ strongly (irreversibly) trapped species

Balance Equations

Balance equations for the mixture mass, the three solute species masses, mixture linear momentum and moment of momentum, mixture energy, and mixture entropy can be written. In this report, our modeling considerations will be restricted to isothermal linear elastic mixtures so that only the balance equations for the solute species mass and mixture linear momentum need be explicitly considered. Assuming negligible inertial effects, they are given by:

Mass :
$$\frac{\partial c_k}{\partial t} + \vec{\nabla} \cdot \vec{\mathcal{J}}_k = a_k \qquad (k = L,\ R,\ or\ I) \tag{1}$$

Linear Momentum:
$$\sigma_{ij,j} + F_i = 0 \qquad (i, j = x,\ y,\ or\ z) \tag{2}$$

where: $c_k \equiv$ mass fraction concentrations for S_k $[kg/kg]$.
$\vec{\mathcal{J}}_k \equiv$ concentration flux vectors for S_k $[kg/kg \cdot m/s]$.
$a_k \equiv$ mass supply rates for S_k $[kg/kg/s]$.
$\sigma_{ij} \equiv$ stress tensor $[N/m^2]$.
$F_i \equiv$ the i^{th} component of body force vector $[N/m^3]$.

Trapping Analysis

Expressions for the mass supply rates a_k in Eq. (1) are written in accordance with the trapping model of McNabb & Foster [11]:

Stoichiometry: $$S_L \Leftrightarrow S_R \quad \text{and} \quad S_L \Rightarrow S_I \tag{3}$$

The stoichiometric relations require the supply terms sum to zero (i.e., $a_R + a_I = -a_L$).

Kinetics of Trapping: $$a_R = k_R^f(1-\theta_{_R})c_L - k_R^b\theta_{_R} \tag{4}$$
$$a_I = k_I^f(1-\theta_{_I})c_L - k_I^b\theta_{_I} \approx k_I^f(1-\theta_{_I})c_L$$

where: k_R^f, k_I^f, k_R^b, $k_I^b \equiv$ forward and backward trap rate constants for S_R and S_I $[1/s]$.
$\theta_{_R}$ and $\theta_{_I} \equiv c_R/c_R^s$ and c_I/c_I^s, respectively, are the fraction of filled trap sites [1].
c_R^s and $c_I^s \equiv$ saturation mass fraction concentration of S_R and S_I $[kg/kg]$.

The quantities k_R^f, k_I^f, k_R^b, k_I^b, c_R^s and c_I^s are related to trap site densities, probability of capture, etc. and can be quantified via experimental measurement (see, for example, [12-14]).

Significant simplifications are effected when the rate constants for trapping are much greater than those for diffusive transport. Trapping can then be modeled as a steady-state process (i.e., $a_L = a_R = a_I = 0$). This case is considered below.

SS Trapping: $$c_R = \frac{c_R^s\, K_R\, c_L}{1 + K_R\, c_L} \approx c_R^s\, K_R\, c_L \quad \& \quad c_I = c_I^s \tag{5}$$
$$K_R \equiv \frac{k_R^f}{k_R^b} = \exp\left(\frac{-\Delta E_b}{\mathbb{R}\,T}\right)$$

The total internal solute concentration is simply a linear function of $c_L(x_i,t)$:

$$c_{TOTAL}(x_i,t) = c_L(x_i,t) + c_R(x_i,t) + c_I(x_i,t) = (1 + c_R^s\, K_R)c_L(x_i,t) + c_I^s \tag{6}$$

The three versions of Eq. (1) (one for each species) can be summed to give a single equation by the following considerations. First, $\vec{\mathcal{J}}_R = \vec{\mathcal{J}}_I = 0$ because of the linear elastic material assumption which precludes trap site motion (e.g., dislocation motion during plastic deformation). Second, from Eq. (5a):

$$\frac{\partial c_R}{\partial t} \approx c_R^s\, K_R\, \frac{\partial c_L}{\partial t} \quad \text{and} \quad \frac{\partial c_I}{\partial t} = 0 \tag{7}$$

Summation of the three balances results in the following single mass balance equation:

$$(1 + c_R^s\, K_R)\frac{\partial c_L}{\partial t} + \vec{\nabla}\cdot\vec{\mathcal{J}}_L = 0 \tag{8}$$

Constitutive Equations

Mass Flux: $$\vec{\mathcal{J}}_L = -\frac{c_L\, D_L}{R_L\, T}\vec{\nabla}\mu_L \quad \textit{Linear Onsager Relation} \tag{9}$$

where μ_L is a *mass* based chemical potential [15] defined by:

$$\mu_L \equiv \frac{\partial \psi}{\partial c_L} = \frac{1}{\mathcal{M}_L}\left(\mu_L^o(T) + \mathbb{R}T\ln(c_L) - \overline{V}_s k e\right) \qquad \left[\frac{J}{kg}\right] \tag{10}$$

and: $D_L \equiv$ diffusion coefficient for S_L $[m^2/s]$.

$R_L \equiv$ gas constant for $S_L = \mathbb{R}/\mathcal{M}_L$ $[J/kg \cdot {}^\circ K]$.

$\mathcal{M}_L \equiv$ molecular mass of S_L $[kg/mol]$.

$T \equiv$ temperature $[^\circ K]$.

$\psi \equiv \psi(c_L,\, c_R,\, c_I; \epsilon_{ij}\,;\, T)$ free energy per unit mixture mass $[J/kg]$.

$\mu_L^o(T) \equiv$ reference potential for S_L at temperature T $[J/mol]$.

$\overline{V}_s \equiv$ partial molar volume of solute in the metal $[m^3/mol\, S]$.

$k \equiv$ bulk modulus of elasticity $[N/m^2]$.

$e \equiv$ trace of the strain tensor (i.e., $e = \epsilon_{ii} = \epsilon_{11} + \epsilon_{22} + \epsilon_{33}$) $[m/m]$.

The use of a mass based chemical potential simplifies the analysis of fully coupled deformation-diffusion processes because of the primary role played by mass in the deformation equations.

The resulting expression for concentration flux is given by:

$$\vec{\mathcal{J}}_L = -D_L \vec{\nabla} c_L + \frac{\overline{V}_s\, D_L}{\mathbb{R}T}\, k c_L \vec{\nabla} e \tag{11}$$

The constitutive equation for the stress consists of Hooke's law combined with a dilatational stress contribution due to changes in the total solute concentration:

Stress:
$$\sigma_{ij} \equiv \rho\, \frac{\partial \psi}{\partial \epsilon_{ij}} = \lambda\, e\, \delta_{ij} + 2G\epsilon_{ij} - 3k\, \alpha_s\, (1 + c_R^s K_R)\, \Delta c_L\, \delta_{ij} \tag{12}$$

where: $\rho \equiv$ mass density of the solid $\left[kg/m^3\right]$.

$\lambda \equiv$ Lame´ constant $[N/m^2]$.

$\delta_{ij} \equiv$ Kronecker delta ($\delta_{ij} = 1$ for $i = j$ and 0 otherwise).

$G \equiv$ shear modulus $[N/m^2]$.

$\epsilon_{ij} \equiv \frac{1}{2}\,(u_{i,j} + u_{j,i})$ infinitesimal strain tensor $[m/m]$.

$u_i \equiv$ the i^{th} component of the displacement vector $[m]$.

$\alpha_s \equiv$ linear expansion coefficient for internal solute $= \frac{1}{3}\frac{\rho}{\mathcal{M}_L}\overline{V}_s$ $[m/m/\Delta c_s]$.

$\Delta c_L \equiv c_L - c_0 =$ change in c_L from the reference level, c_0.

$(1 + c_R^s K_R)\Delta c_L \equiv$ change in c_{total} from the reference level.

The influence of the irreversibly trapped solute on the deformation of the solid has been ignored in Eq. (12). The assumption of equilibrium trapping implies that $c_I \rightarrow c_I^s$ immediately upon introducing solute into the solid. We have assumed, therefore, that $c_I = c_I^s$, and that all deformations are measured with respect to an initial uniform deformation arising from the presence of the irreversibly trapped solute species at its saturation concentration level.

The relationship between the chemical potential and stress (Eqs. (10) and (12)) is dictated by the thermodynamic reciprocity relationship:

$$\frac{\partial \mu_L}{\partial \epsilon_{ij}} = \frac{\partial (\sigma_{ij}/\rho)}{\partial c_L} \tag{13}$$

The equations of classical stress assisted diffusion violate this requirement by ignoring the concentration induced dilatational stresses.

Governing Equations

Combining the mass and momentum balance equations with the constitutive relations results in the following system of governing equations for transport:

Diffusion Equation:

$$\frac{\partial c_L}{\partial t} = D_{eff}\,\nabla^2 c_L - \frac{\overline{V}_s\, D_{eff}}{\mathbb{R}\,T} k \Big(\vec{\nabla} c_L \cdot \vec{\nabla} e + c_L \nabla^2 e \Big) \tag{14}$$

Deformation Equations ($i = 1,\ 2,\ 3$):

$$(\lambda + G)\frac{\partial e}{\partial x_i} + G\,\nabla^2 u_i + F_i = 3k\,\alpha_s (1 + c_R^s K_R)\frac{\partial c_L}{\partial x_i} \tag{15}$$

where D_{eff} is an "effective" diffusion coefficient defined by: $D_{eff} \equiv D_L/(1 + c_R^s K_R)$.

Equation (14) is identical to the SAD equations published in the literature with the exception of the $\nabla^2 e$ term which is identically zero when linear elastic material behavior is assumed (no coupling and $F_i = 0$). In the present formulation it is given by:

$$\nabla^2 e = \frac{3k\,\alpha_s}{\lambda + 2G}(1 + c_R^s\ K_R)\nabla^2 c_L \tag{16}$$

FINITE ELEMENT MODELING

Equations (14) and (15) form a system of non-linearly coupled partial differential equations that must be solved for c_L and u_i as functions of the space and time coordinates (x_i, t). In developing the finite element equations, it is more convenient to work with the system of balance equations joined with appropriate constitutive equations. The 1-D form of the equations, with both "plane stress" and "plane strain" constitutive relations, is given by:

Diffusion:

$$\frac{\partial c_L}{\partial t} + \frac{\partial \mathcal{J}_L^*}{\partial x} = 0 \tag{17}$$

$$\mathcal{J}_L^* \equiv -\,D_{eff}\frac{\partial c_L}{\partial x} + \frac{\overline{V}_s\, D_{eff}}{\mathbb{R}\,T}\, k c_L \frac{\partial e}{\partial x}$$

Deformation:

$$\frac{\partial \sigma_x}{\partial x} + F_x = 0 \tag{18}$$

Plane Stress Constitutive Relations: $(\sigma_y, \sigma_z, \sigma_{xy}, \sigma_{yz}, \sigma_{zx} = 0)$

$$\sigma_x = 3ke - 9k\alpha_s(1 + c_R^s K_R)\Delta c_L = E\epsilon_x - E\alpha_s(1 + c_R^s K_R)\Delta c_L \tag{19}$$

Plane Strain Constitutive Relations: $(\epsilon_y, \epsilon_z, \epsilon_{xy}, \epsilon_{yz}, \epsilon_{zx} = 0)$

$$\begin{aligned} \sigma_x &= (\lambda + 2G)e - 3k\alpha_s(1 + c_R^s K_R)\Delta c_L \\ &= \frac{E\,(1-\nu)}{(1-2\nu)(1+\nu)}\epsilon_x - \frac{E}{(1-2\nu)}\alpha_s(1 + c_R^s K_R)\Delta c_L \end{aligned} \tag{20}$$

A single differential equation for c_L, under plane stress conditions, can be obtained using Eqs. (17) through (19):

$$\frac{\partial c_L}{\partial t} = \frac{\partial}{\partial x}\left[D_{eff}\left(1 - \frac{\rho\,\overline{V}_s^{\,2}\,k}{\mathcal{M}_L\,\mathbb{R}\,T}(1 + c_R^s\,K_R)c_L\right)\frac{\partial c_L}{\partial x} + \frac{\overline{V}_s\,D_{eff}}{3\,\mathbb{R}\,T}F_x c_L\right] \tag{21}$$

In the absence of body forces, this is a standard diffusion equation with a concentration dependent diffusion coefficient. Solutions to the steady-state problem, with and without body forces, can be obtained straightforwardly by integration; symbolic computation is recommended (see Appendix A).

Programming Simplifications

The following generalizations are made to the expressions for dilatational strain e and axial stress σ_x to simplify the subsequent finite element coding. They are obtained using Eqs. (19) and (20) and the definition for Δc_L:

$$\begin{aligned} e &= A_1\frac{\partial u}{\partial x} + A_2 c_L - A_3 \\ \sigma_x &= B_1 e - B_2 c_L + B_3 \end{aligned} \tag{22}$$

where A_i and B_i $(i = 1, 2, \text{ or } 3)$ are constants defined in the table below:

Constant	*Plane Stress*	*Plane Strain*
A_1	$(1-2\nu)$	1
A_2	$2(1+\nu)\alpha_s(1 + c_r^s K_r)$	0
A_3	$A_2 \times c_0$	0
B_1	$3k$	$(\lambda + 2G)$
B_2	$9k\alpha_s(1 + c_r^s K_r)$	$3k\alpha_s(1 + c_r^s K_r)$
B_3	$B_2 \times c_0$	$B_2 \times c_0$

Table 1: Constants for the dilatational strain, e, and axial stress, σ_x, relations.

The elastic constants needed as input to the finite element program are the elastic modulus, E, and Poisson's ratio, ν. Conversions from bulk modulus, k, and $\lambda + 2G$ (λ = Lamé constant and G = shear modulus) are given by:

$$k = \frac{E}{3(1-2\nu)} \tag{23}$$
$$\lambda + 2G = \frac{(1-\nu)E}{(1+\nu)(1-2\nu)}$$

The equations of classical stress assisted diffusion result by setting the constants A_2, A_3, B_2, and B_3 equal to zero.

Formulation of the Finite Element Matrix Equations

Galerkin method of weighted residuals is used to formulate the finite element matrix equations. This procedure uses the interpolation functions as weights in the integral formulation given below [16]:

$$\int_{V_e} \left(\frac{\partial c_L}{\partial t} + \frac{\partial \mathcal{J}_L^*}{\partial x} \right) G_i \, dV_e = 0 \tag{24}$$
$$\int_{V_e} \left(\frac{\partial \sigma_x}{\partial x} + F_x \right) H_j \, dV_e = 0$$

where: $G_i \equiv i^{th}$ concentration interpolation function, $(G_i = G_i(x))$.
$H_j \equiv j^{th}$ displacement interpolation function, $(H_j = H_j(x))$.
$dV_e \equiv$ differential element volume $= A_e dx$.
$A_e \equiv$ cross-sectional area $(A_e = A_e(x))$.

Integrating the second term of Eq.(24a) and the first term of Eq.(24b) by parts yields the coupled set of equations for a single finite element of length h $(0 \leq x \leq h)$:

$$\int_0^h \left(\frac{\partial c_L}{\partial t} \{G_i(x)\} - \mathcal{J}_L^* \left\{ \frac{\partial G_i(x)}{\partial x} \right\} \right) A_e \, dx = -A_e \mathcal{J}_L^* \{G_i(x)\} \Big|_0^h \tag{25}$$
$$\int_0^h \left(-\sigma_x \left\{ \frac{\partial H_j(x)}{\partial x} \right\} + F_x \{H_j(x)\} \right) A_e \, dx = -A_e \sigma_x \{H_j(x)\} \Big|_0^h$$

The RHS term $A_e \mathcal{J}_L^*$ represents the axial solute influx through the element boundaries and $A_e \sigma_x$ represents the axial force applied at each end of the element.

Interpolation Functions for the Concentration and Displacement

The concentration is represented using a linear interpolation function, and the displacement is represented using a quadratic interpolation function:

$$c_L \equiv \sum_{i=1}^{2} G_i(x) c_i(t) = \lfloor G_i(x) \rfloor \{c_i(t)\} \qquad i = 1,2 \tag{26}$$

$$\frac{\partial c_L}{\partial x} \equiv \sum_{i=1}^{2} \frac{dG_i(x)}{dx} c_i(t) = \left\lfloor \frac{dG_i(x)}{dx} \right\rfloor \{c_i(t)\} \qquad i = 1,2$$

$$\frac{\partial c_L}{\partial t} \equiv \sum_{i=1}^{2} G_i(x) \frac{dc_i(t)}{dt} = \lfloor G_i(x) \rfloor \left\{ \frac{dc_i(t)}{dt} \right\} \qquad i = 1,2$$

$$u \equiv \sum_{j=1}^{3} H_j(x) u_j(t) = \lfloor H_j(x) \rfloor \{u_j(t)\} \qquad j = 1,2,3 \tag{27}$$

$$\frac{\partial u}{\partial x} \equiv \sum_{j=1}^{3} \frac{dH_j(x)}{dx} u_j(t) = \left\lfloor \frac{dH_j(x)}{dx} \right\rfloor \{u_j(t)\} \qquad j = 1,2,3$$

$$\frac{\partial u}{\partial t} \equiv \sum_{j=1}^{3} H_j(x) \frac{du_j(t)}{dt} = \lfloor H_j(x) \rfloor \left\{ \frac{du_j(t)}{dt} \right\} \qquad j = 1,2,3$$

where $\lfloor \cdots \rfloor$ indicates a row matrix and $\{\cdots\}$ a column matrix. Substitution of these into Eqs.(22a,b) and (17b) for the dilatational strain, stress, and mass flux, respectively, give:

$$e = A_1 \left\lfloor \frac{dH_j(x)}{dx} \right\rfloor \{u_j(t)\} + A_2 \lfloor G_i(x) \rfloor \{c_i(t)\} - A_3 \tag{28}$$

$$\sigma_x = B_1 A_1 \left\lfloor \frac{dH_j(x)}{dx} \right\rfloor \{u_j(t)\} + (B_1 A_2 - B_2) \lfloor G_i(x) \rfloor \{c_i(t)\} + (B_3 - B_1 A_3)$$

$$\mathcal{J}_L^* = -D_{eff} \left\lfloor \frac{dG_i(x)}{dx} \right\rfloor \{c_i(t)\} + D_{eff}\, K_1 \lfloor G_i(x) \rfloor \{c_i(t)\} \frac{\partial e}{\partial x}$$

Substituting Eqs.(28a,b,c) into Eq.(25a,b) and collecting terms in $\{c_i(t)\}$, $\{u_i(t)\}$, $\{\dot{c}_i(t)\}$, and $\{\dot{u}_j(t)\}$ yields the following matrix equation:

$$\begin{bmatrix} [C_c] & [0] \\ [0] & [0] \end{bmatrix} \begin{Bmatrix} \{\dot{c}_i\} \\ \{\dot{u}_j\} \end{Bmatrix} + \begin{bmatrix} [K_c] & [K_{cu}] \\ [K_{uc}] & [K_u] \end{bmatrix} \begin{Bmatrix} \{c_i\} \\ \{u_j\} \end{Bmatrix} = \begin{Bmatrix} \{R_c\} \\ \{R_u\} \end{Bmatrix} \tag{29}$$

where:

$$\{\dot{c}_i\} \equiv \frac{dc_i}{dt} \tag{30}$$

$$\{\dot{u}_i\} \equiv \frac{du_i}{dt}$$

$$[C_c] \equiv A_e \int_0^h \{G_i(x)\} \lfloor G_i(x) \rfloor dx \tag{31}$$

$$[K_{cu}] \equiv [0] \tag{32}$$

$$[K_u] \equiv A_e \int_0^h B_1 A_1 \left\{ \frac{dH_j(x)}{dx} \right\} \left\lfloor \frac{dH_j(x)}{dx} \right\rfloor dx$$

$$[K_{uc}] \equiv A_e \int_0^h (B_1 A_2 - B_2) \left\{ \frac{dH_j(x)}{dx} \right\} \lfloor G_i(x) \rfloor dx$$

$$[K_c] \equiv A_e \int_0^h D_{eff} \left(\left\{ \frac{dG_i(x)}{dx} \right\} \left\lfloor \frac{dG_i(x)}{dx} \right\rfloor - K_1 \left\{ \frac{dG_i(x)}{dx} \right\} \frac{\partial e}{\partial x} \lfloor G_i(x) \rfloor \right) dx$$

$$\{R_c\} \equiv -A_e \mathcal{J}_L^* \{G_i(x)\} \Big|_0^h \tag{33}$$

$$\{R_u\} \equiv A_e \int_0^h \left(\{H_j(x)\} F_x - (B_3 - B_1 A_3) \left\{ \frac{dH_j(x)}{dx} \right\} \right) dx + A_e \sigma_x \{H_j(x)\} \Big|_0^h$$

and where the cross-sectional area, A_e, is assumed to be constant within the element.

The fact that $[K_{cu}]$ is zero might appear to imply that there is no coupling between concentration and deformation, but this is not the case. The $[K_c]$ contains the first derivative of the hydrostatic strain, $\partial e/\partial x$, which contains, in turn, the second derivative in the displacement, u (from Eq. (22a)):

$$\frac{\partial e}{\partial x} = A_1 \frac{\partial^2 u}{\partial x^2} + A_2 \frac{\partial c_L}{\partial x} \tag{34}$$

The presence of the second order derivative in u would normally require the use of C^1 continuous elements in order for u to satisfy element interface compatibility requirements [16]. To avoid this complication, the values of u and c_L from the previous time step are used to approximate $\partial e/\partial x$ for the current time calculations.

The integral expressions in Eqs. (31) through (33) use interpolation functions expressed in terms of the global coordinate, x. The code will be implemented using isoparametric coordinates[4] which requires replacement of the functions $G_i(x)$ and $H_j(x)$ by an appropriate set of isoparametric interpolation functions.

Isoparametric Interpolation Functions

Standard linear and quadratic isoparametric interpolation functions, expressed in terms of the local coordinate r ($-1 \leq r \leq 1$) are given by [17]:

$$g_1(r) \equiv \frac{1}{2}(1-r), \quad g_2(r) \equiv \frac{1}{2}(1+r) \tag{35}$$

$$h_1(r) \equiv \frac{1}{2}\left(r^2 - r\right), \quad h_2(r) \equiv \left(1 - r^2\right), \quad h_3(r) \equiv \frac{1}{2}\left(r^2 + r\right)$$

[4] The transformation from global to local coordinates is *isoparametric* in displacement and *superparametric* in concentration. The term isoparametric will be used here to refer to the local coordinate parametrization of the element geometry which extends from -1 at the left-hand end of the element to +1 at the right-hand end.

For an element with the global node locations, x_i, the correspondence between the global coordinate, x, and the local coordinate, r, is given by the transformation:

$$x = \lfloor h_j(r) \rfloor \{x_j\} \tag{36}$$

Equations (31) through (33) can now be expressed in terms of the local r coordinates via the following substitutions:

$$\begin{gathered} \{H_j(x)\} \mapsto \{h_j(r)\}, \quad \{G_i(x)\} \mapsto \{g_i(r)\} \\ \left\{ \frac{dH_j(x)}{dx} \right\} \mapsto [\, J^{-1}] \left\{ \frac{dh_j(r)}{dr} \right\}, \quad \left\{ \frac{dG_i(x)}{dx} \right\} \mapsto [\, J^{-1}] \left\{ \frac{dg_i(r)}{dr} \right\} \\ \int_0^h dx \mapsto \int_{-1}^{+1} | \, J \, | dr \end{gathered} \tag{37}$$

where:

$$[\, J \,] \equiv \left[\frac{dx}{dr} \right] = \left\lfloor \frac{dh_j(r)}{dr} \right\rfloor \{x_j\} = \left(r - \frac{1}{2} \right) x_1 - (2\, r)\, x_2 + \left(r + \frac{1}{2} \right) x_3 \tag{38}$$

is the "scalar" Jacobian transformation matrix, J, with determinant $| \, J \, | = J$, and inverse $[\, J^{-1} \,] = \frac{1}{J}$. Using Eqs.(36) through (38) in Eqs. (29), (30), and (33) yields the following relations:

$$[C_c] \equiv A_e \int_{-1}^{+1} \{g_i(r)\} \lfloor g_i(r) \rfloor J \, dr \tag{39}$$

$$\begin{gathered} [K_{cu}] \equiv [0] \\ [K_u] \equiv A_e \int_{-1}^{+1} B_1 A_1 \left\{ \frac{dh_j(r)}{dr} \right\} \left\lfloor \frac{dh_j(r)}{dr} \right\rfloor \frac{1}{J} \, dr \\ [K_{uc}] \equiv A_e \int_{-1}^{+1} (B_1 A_2 - B_2) \left\{ \frac{dh_j(r)}{dr} \right\} \lfloor g_i(r) \rfloor \, dr \\ [K_c] \equiv A_e \int_{-1}^{+1} D_{eff} \left(\left\{ \frac{dg_i(r)}{dr} \right\} \left\lfloor \frac{dg_i(r)}{dr} \right\rfloor - K_1 \left\{ \frac{dg_i(r)}{dr} \right\} \frac{\partial e}{\partial r} \lfloor g_i(r) \rfloor \right) \frac{1}{J} \, dr \end{gathered} \tag{40}$$

$$\begin{gathered} \{R_c\} \equiv \, - A_e \, \mathcal{J}_L^* \, \{g_i(r)\} \Big|_{-1}^{+1} \\ \{R_u\} \equiv A_e \int_{-1}^{+1} \left(\{h_j(r)\} F_x \, - (B_3 - B_1 A_3) \frac{1}{J} \left\{ \frac{dh_j(r)}{dr} \right\} \right) J \, dr \, + A_e \sigma_x \{h_j(r)\} \Big|_{-1}^{+1} \end{gathered} \tag{41}$$

and $\partial e / \partial x$ in $[K_c]$ has been replaced with $(\partial e / \partial r)/J$ via use of the chain-rule of differentiation.

Gauss-Legendre Numerical Integration

The above integrals are evaluated using a Gauss-Legendre numerical integration scheme. The variable r occurs as a $3rd$ degree quantity in the expression for $[K_{uc}]$. A two-

point integration using Gauss-point locations, $r_k = \pm 1/\sqrt{3}$, and Gauss weights, $W_k = 1.0$ is therefore selected for use in the numerical calculations [16,17]:

$$[C_c] \equiv \sum_{k=1}^{2} A_e W_k \, J(r_k) \{g_i(r_k)\} \lfloor g_i(r_k) \rfloor \tag{42}$$

$$[K_{cu}] \equiv [0] \tag{43}$$

$$[K_u] \equiv \sum_{k=1}^{2} \frac{A_e W_k \, B_1 \, A_1}{J(r_k)} \left\{ \frac{dh_j(r_k)}{dr} \right\} \left\lfloor \frac{dh_j(r_k)}{dr} \right\rfloor$$

$$[K_{uc}] \equiv \sum_{k=1}^{2} A_e W_k (B_1 \, A_2 - B_2) \left\{ \frac{dh_j(r_k)}{dr} \right\} \lfloor g_i(r_k) \rfloor$$

$$[K_c] = \sum_{k=1}^{2} \frac{A_e W_k \, D_{eff}}{J(r_k)} \left(\left\{ \frac{dg_i(r_k)}{dr} \right\} \left\lfloor \frac{dg_i(r_k)}{dr} \right\rfloor - K_1 \frac{de}{dr} \left\{ \frac{dg_i(r_k)}{dr} \right\} \lfloor g_i(r_k) \rfloor \right)$$

$$\{R_c\} \equiv - A_e \mathcal{J}_L^* \{g_i(r)\} \Big|_{-1}^{+1} \tag{44}$$

$$\{R_u\} \equiv \sum_{k=1}^{2} A_e W_k \left(J(r_k) F_x \{h_j(r_k)\} - (B_3 - B_1 A_3) \left\{ \frac{dh_j(r_k)}{dr} \right\} \right) + A_e \sigma_x \{h_j(r)\} \Big|_{-1}^{+1}$$

Finite Element Equations

The matrix finite element equations given by Eq. (29) are rewritten, following reference [16], in the form:

$$[C(v_\theta)]\{\dot{v}\}_\theta + [K(v_\theta)]\{v\}_\theta = \{R(t_\theta)\} \tag{45}$$

where $\{v\}$ is the vector of nodal degrees of freedom and θ $(0 \leq \theta \leq 1)$ parameterizes the time integration scheme via the following definitions:

$$\begin{aligned} t_\theta &\equiv t_n + \theta \Delta t \\ \{v\}_\theta &\equiv (1-\theta)\{v\}_n + \theta \{v\}_{n+1} \\ \{\dot{v}\}_\theta &\equiv \frac{\{v\}_{n+1} - \{v\}_n}{\Delta t} \end{aligned} \tag{46}$$

For $\theta = 0$ and a lumped capacitance matrix, the algorithm is explicit; for $\theta = \frac{1}{2}$, the algorithm is Crank-Nicolson; for $\theta = \frac{2}{3}$ the algorithm is Galerkin; and for $\theta = 1$, the algorithm is the backward difference.

The coupled temperature-displacement solver routine in ABAQUS is used to solve the fully coupled system of transport equations represented by Eq. (45). This particular ABAQUS routine uses the backward difference algorithm for time integration. Substituting $\theta = 1$ into Eqs. (46) gives:

$$t_{\theta=1} = t_{n+1} = t_n + \Delta t \tag{47}$$
$$\{v\}_{\theta=1} = \{v\}_{n+1}$$
$$\{\dot{v}\}_{\theta=1} = \{\dot{v}\}_{n+1} = \frac{\{v\}_{n+1} - \{v\}_n}{\Delta t}$$

which, when substituted into Eq.(45) yields:

$$\left[[\mathcal{K}(v_{n+1})] + \frac{[\mathcal{C}(v_{n+1})]}{\Delta t}\right]\{v\}_{n+1} = \frac{[\mathcal{C}(v_{n+1})]}{\Delta t}\{v\}_n + \{\mathcal{R}(t_{n+1})\} \tag{48}$$

If $[\mathcal{C}]$ and $[\mathcal{K}]$ are independent of the degrees of freedom $\{v\}$, then the problem is linear, and the equations may be solved directly for $\{v\}_{n+1}$ via standard linear systems solver routines. On the other hand, if $[\mathcal{C}]$ or $[\mathcal{K}]$ is a function of v, then Eq. (48) is non-linear and must be solved using more specialized techniques. One of the techniques used by ABAQUS is the Newton-Raphson method. It is described below.

Non-Linear Solutions via Newton-Raphson

Assume that $\{v\}_n$ is known and we wish to determine $\{v\}_{n+1}$. First, define the "residual" vector $\{f(v_{n+1})\}$:

$$\{f(v_{n+1})\} \equiv -\left[[\mathcal{K}(v_{n+1})] + \frac{[\mathcal{C}(v_{n+1})]}{\Delta t}\right]\{v\}_{n+1} + \frac{[\mathcal{C}(v_{n+1})]}{\Delta t}\{v\}_n + \{\mathcal{R}(t_{n+1})\} \tag{49}$$

where $\{f(v_{n+1})\} = \{0\}$ for a $\{v\}_{n+1}$ which is a solution to Eq. (48). Defining $\{v\}^i_{n+1}$ as the i^{th} iterated approximation to the actual solution, $\{v\}_{n+1}$, leads to the following definition for the $(i+1)^{st}$ iterated approximation:

$$\{v\}^{i+1}_{n+1} \equiv \{v\}^i_{n+1} + \{\Delta v\}^{i+1}_{n+1} \tag{50}$$

where $\{\Delta v\}^{i+1}_{n+1}$ is a correction vector. This correction vector $\{\Delta v\}^{i+1}_{n+1}$ can be determined by expanding $\{f(v_{n+1})\}$ in a Taylor's series approximation about the point $\{v\}^i_{n+1}$, retaining only the zeroth and first order terms, and then setting the resulting expression equal to zero:

$$\{f(v^{i+1}_{n+1})\} \approx \{f(v^i_{n+1})\} + \left.\frac{\partial\{f(v^i_{n+1})\}}{\partial\{v\}^i_{n+1}}\right|_{\{v\}^i_{n+1}} \{\Delta v\}^{i+1}_{n+1} = \{0\} \tag{51}$$

Now,

$$\frac{\partial\{f(v^i_{n+1})\}}{\partial\{v\}^i_{n+1}} = -\left[[\mathcal{K}(v^i_{n+1})] + \frac{[\mathcal{C}(v^i_{n+1})]}{\Delta t}\right] - \left[[\mathcal{K}'(v^i_{n+1})] + \frac{[\mathcal{C}'(v^i_{n+1})]}{\Delta t} - \frac{[\mathcal{C}''(v^i_{n+1})]}{\Delta t}\right] \tag{52}$$

where we have defined:

$$[\mathcal{K}'(v^i_{n+1})] \equiv \left[\frac{\partial[\mathcal{K}(v^i_{n+1})]}{\partial\{v\}^i_{n+1}}\right]\{v\}^i_{n+1} \tag{53}$$

$$[\mathcal{C}'(v^i_{n+1})] \equiv \left[\frac{\partial[\mathcal{C}(v^i_{n+1})]}{\partial\{v\}^i_{n+1}}\right]\{v\}^i_{n+1}$$

$$[\mathcal{C}''(v^i_{n+1})] \equiv \left[\frac{\partial[\mathcal{C}(v^i_{n+1})]}{\partial\{v\}^i_{n+1}}\right]\{v\}^i_{n}$$

Now define:
$$[\Delta\mathcal{C}'(v^i_{n+1})] \equiv [\mathcal{C}'(v^i_{n+1})] - [\mathcal{C}''(v^i_{n+1})] \tag{54}$$

then:
$$\frac{\partial\{f(v^i_{n+1})\}}{\partial\{v\}^i_{n+1}} = -\left[[\mathcal{K}(v^i_{n+1})] + \frac{[\mathcal{C}(v^i_{n+1})]}{\Delta t}\right] - \left[[\mathcal{K}'(v^i_{n+1})] + \frac{[\Delta\mathcal{C}'(v^i_{n+1})]}{\Delta t}\right] \tag{55}$$

A simplification used in the numerical computations is to assume that $[\mathcal{K}']$ and $[\Delta\mathcal{C}']$ are approximately zero. This results in significant computational savings but reduces the convergence speed for the interative solution. Eq. (55) defines the 5×5 "Jacobian" matrix denoted in ABAQUS by "$AMATRX$".

Re-ordering the Degrees of Freedom

The ordering of the degrees of freedom (dof) in the system matrix equation, Eq. (29) or (45), violates the ABAQUS convention which groups the degrees of freedom by node [18]. The current layout of $[\mathcal{K}]$ in Eq. (45) is given by:

$$\begin{bmatrix} [K_c] & [K_{cu}] \\ [K_{uc}] & [K_u] \end{bmatrix} = \begin{bmatrix} [K_c] & [0] \\ [K_{uc}] & [K_u] \end{bmatrix} = \begin{bmatrix} K_c^{11} & K_c^{12} & 0 & 0 & 0 \\ K_c^{21} & K_c^{22} & 0 & 0 & 0 \\ K_{uc}^{11} & K_{uc}^{12} & K_u^{11} & K_u^{12} & K_u^{13} \\ K_{uc}^{21} & K_{uc}^{22} & K_u^{21} & K_u^{22} & K_u^{23} \\ K_{uc}^{31} & K_{uc}^{32} & K_u^{31} & K_u^{32} & K_u^{33} \end{bmatrix} \tag{56}$$

a non-sparse block matrix. Rearranging the order of the dof's to conform with the ABAQUS convention requires:

$$\{v\} = \begin{Bmatrix} c_1 \\ u_1 \\ u_2 \\ c_3 \\ u_3 \end{Bmatrix} \tag{57}$$

This reordering gives the new element stiffness matrix layout:

$$[\mathcal{K}] = \begin{bmatrix} K_c^{11} & 0 & 0 & K_c^{12} & 0 \\ K_{uc}^{11} & K_u^{11} & K_u^{12} & K_{uc}^{12} & K_u^{13} \\ K_{uc}^{21} & K_u^{21} & K_u^{22} & K_{uc}^{22} & K_u^{23} \\ K_c^{21} & 0 & 0 & K_c^{22} & 0 \\ K_{uc}^{31} & K_u^{31} & K_u^{32} & K_{uc}^{32} & K_u^{33} \end{bmatrix} \tag{58}$$

The capacitance matrix must also be altered to reflect the new ordering given by Eq. (57).

ABAQUS User Element Subroutines

ABAQUS executes a Fortran subroutine named UEL for each "user defined" finite element in the model. Current values for the: **1.** material properties; **2.** total and incremental nodal degrees of freedom; **3.** time incrementation parameters; and **4.** user-defined state variables (i.e., the dilatational strain and axial stress at the Gauss integration points; extrapolated axial stress at the element boundaries; the mass flux at the center of the element; and the Gauss point locations) are passed from the main ABAQUS code into the UEL. Depending on the exact stage in the time increment, the subroutine UEL must return some combination of the: "Jacobian" matrix ($AMATRX$); right-hand side vector (RHS); and updated values of the state variables.

From Eq.(51), we have:

$$\left.\frac{\partial\{f(v_{n+1}^i)\}}{\partial\{v\}_{n+1}^i}\right|_{\{v\}_{n+1}^i} \{\Delta v\}_{n+1}^{i+1} = -\{f(v_{n+1}^i)\} \tag{59}$$

or

$$AMATRX\,\{\Delta v\}_{n+1}^{i+1} = -RHS \tag{60}$$

where

$$AMATRX \approx \frac{1}{\Delta t}\left[\mathcal{C}(v_{n+1}^i)\right] + \left[\mathcal{K}(v_{n+1}^i)\right] \tag{61}$$

and

$$RHS = \{\mathcal{R}\} - [\mathcal{K}]\{v\}_{n+1}^i - \frac{1}{\Delta t}[\mathcal{C}]\{\Delta v\}_{n+1}^i \tag{62}$$

On return from subroutine UEL, ABAQUS assembles the $AMATRX$ and RHS from each element into the global matrix equation:

$$[AMATRX]_G\{\Delta v\}_{n+1}^{i+1} = \{RHS\}_G \tag{63}$$

and adds contributions from concentrated loads into the RHS array. ABAQUS solves Eq. (63) for the incremental correction $\{\Delta v\}_{n+1}^{i+1}$ using standard solution techniques. The solution process is repeated until the residual, that is, the $\{RHS\}_G$ vector, is smaller than some specified tolerance, at which point the solution is accepted as correct. The tolerances used with this UEL subroutine must typically be set in the ABAQUS input deck, since the residuals for the displacement and concentration variables generally show many orders of magnitude difference.

MODELING APPLICATIONS

A variety of one-dimensional hydrogen transport problems have been used to explore the differences between the fully coupled transport theory, described in this paper, and classical SAD theory. Analytical and finite element solutions for the steady-state distributions of: hydrogen, axial stress, axial and dilatational strains, and the axial displacement have been obtained for a ($10\,cm \times 1.0\,cm^2$) cylindrical rod of 4340 steel subjected to various boundary conditions and applied body forces. Plane stress conditions are assumed for all problems.

The boundary conditions consist of concentration or mass flux and displacement or load (stresses) at each end of the rod. The analytical solutions are obtained using the Maple symbolic computation program, and the numerical solutions are obtained using ABAQUS with our custom Fortran user element subroutine. The problems examined both analytically and numerically are summarized in Table 2. Other problems that have been examined analytically are documented in Appendix A.

Case #	*Deformation Boundary Conditions*		*Diffusion Boundary Conditions*		*Body Force*	*# Elements*
1a	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-6}$	0	10
2a	$u(LHS) = 0.0$	$u(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-6}$	0	10
3 (LT)	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	$\frac{15\times10^6}{\sqrt{x^3}}$	200
3 (HT)	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	$\frac{15\times10^6}{\sqrt{x^3}}$	200

Table 2: Displacements, u, are specified in $[m]$; loads, P_x, in $[N]$; concentrations, c_L, in $[gH/gFe]$; mass flux, $\mathcal{J}_L$, in $[m/s]$; and body force, F_x, in $[N/m^3]$. Case 3a (LT) and (HT) correspond to low and high trapping ($1 + c_R^s K_R = 20$ and 500).

Case 1 and 2 problems were used to gain insight into the differences between the fully coupled theory, SAD theory, and classical diffusion theory. They also proved useful as benchmark problems for debugging and verifying the user element subroutine.

Case 3 was posed in order to better assess the influence of the hydrogen induced deformations, which are not accounted for in classical SAD theory, at a crack-like stress singularity. A square-root singular stress was introduced in the rod by subjecting it to the fictitious body force:

$$F_x = \frac{15 \times 10^6}{\sqrt{(x+\epsilon)^3}} \tag{64}$$

The variable ϵ is a small constant (2.0×10^{-18}) included to prevent inadvertent Fortran errors at $x = 0$. Substituting this into Eq. (18) and integrating results in the square-root singular stress:

$$\sigma_x = \frac{30 \times 10^6}{\sqrt{x+\epsilon}} \tag{65}$$

The numerator of Eq. (65) is equivalent to a stress-field intensity factor, K, which means that we have adopted a stress-field K value of 30 $[MPa\sqrt{m}]$ for these Case 3 problems.

The introduction of this singularity into the 1-D rod problem resulted in some interesting, but unexpected, behavior in the mathematical solution for the concentration as a

function of x. We found that the concentration becomes a multi-valued function of x as the singularity at $x = 0$ is approached. The exact point at which the concentration becomes multi-valued is predictable and depends only on material constants. Various features of the analytical solution will be discussed in the following Results and Discussion sections, but as a consequence, we have had to modify the rod geometry in our Case 3 numerical analysis so that the left hand boundary starts at $x = 4.0 \times 10^{-5}[m]$ rather than $x = 0$. This avoids the numerical problems associated with multi-valued concentrations.

The material properties used in the analytical and numerical analyses are given below in Table 3:

Property	***Value***
Mass Density, ρ	$7.8\,[g/cm^3]$
Temperature, T	$293\,[K]$
Lattice Diffusion Coefficient[1], D_L	$1 \times 10^{-5}\,[cm^2/s]$
Partial Molar Volume of Hydrogen[2], $\overline{V}_H$	$2.0\,[cm^3/mol]$
Saturation Trapping Concentration[3], c_R^s	2×10^{-12} to $10^{-4}\,[g\,H/g\,Fe]$
Reversible Trap Binding Enthalpy[3], H_B	3.3 to $30\,[kJ/mol]$
$K_R = exp\left(\frac{H_B}{RT}\right)$	4 to 2.2×10^5
Trapping Factor, $(1 + c_R^s K_R)$	20 and 500
Molecular Weight of Hydrogen, $\mathcal{M}_L$	$1.00797\,[g/mol]$
Modulus of Elasticity, E	$200\,[Gpa]$
Poisson's Ratio, ν	0.3
Reference Concentration, c_0	$0\,[g\,H/g\,Fe]$

Table 3: Material property values used in the Maple and finite element analyses.

RESULTS

The results are presented in two subsections. The first subsection corresponds with the Case 1a and 2a problems, and the second subsection corresponds with the Case 3 problem. Each subsection is further divided into parts describing the analytical and finite element solution procedures and description of results.

Case 1 & 2 Problems

Analytical solutions to the 1-D problem can be obtained by solving Eq. (21) for concentration. For the convenience of the reader, Eq. (21) is repeated below:

$$\frac{\partial c_L}{\partial t} = \frac{\partial}{\partial x}\left[D_{eff}\left(1 - \frac{\rho\,\overline{V}_s^{\,2}\,k}{\mathcal{M}_L\,\mathbb{R}\,T}(1 + c_R^s\,K_R)c_L\right)\frac{\partial c_L}{\partial x} + \frac{\overline{V}_s\,D_{eff}}{3\,\mathbb{R}\,T}F_x c_L\right] \qquad (21)$$

[1] Approximate value taken for α-Fe from Figure 12.4 of reference [19].
[2] Approximate value taken from Section III.A.2 of reference [6].
[3] Range of values obtained from Table I of Section III.B.1 of reference [6] with $H_B \leq 30\,[kJ/mol]$.

This is a non-linear diffusion equation with a concentration dependent diffusion coefficient. Under steady state conditions the equation simplifies to:

$$\left(1 - \frac{\rho \overline{V}_s^{\,2} k}{\mathcal{M}_L \mathbb{R} T}(1 + c_R^s K_R) c_L\right) \frac{dc_L}{dx} + \frac{\overline{V}_s}{3\,\mathbb{R}\,T} F_x c_L = Constant \tag{66}$$

where the constant is proportional to the mass flux that obtains under steady-state conditions.

For Cases 1 & 2, the body force, F_x, is also taken to be equal to zero, so that the governing differential equation simplifies to:

$$\left(1 - \frac{\rho \overline{V}_s^{\,2} k}{\mathcal{M}_L \mathbb{R} T}(1 + c_R^s K_R) c_L\right) \frac{dc_L}{dx} = Constant \tag{67}$$

This equation can be integrated to give $c_L(x)$, and once $c_L(x)$ is known, Eq. (18) and (22b) can be combined to give:

$$\frac{de}{dx} = \frac{B_2}{B_1} \frac{dc_L(x)}{dx} \tag{68}$$

This can be integrated using the known function $c_L(x)$ to give the dilatational strain, e, and the axial strain and axial stress can then be obtained directly from Eqs. (22a,b):

$$\epsilon_x = \frac{du}{dx} = \frac{e(x)}{A_1} - \frac{A_2}{A_1} c_L(x) + \frac{A_3}{A_1} \tag{69}$$

$$\sigma_x = B_1 e(x) - B_2 c_L(x) + B_3$$

Finally, the displacement, u, can be obtained by integrating Eq. (69a). The constants of integration in the expressions for: $c_L(x)$, J_L, $e(x)$, $\epsilon_x(x)$, $\sigma_x(x)$, and $u(x)$ can be determined using the given boundary data.

The above steps were performed, in this work, using the Maple V symbolic computation program on a Sun SPARC10 workstation. The general results are given below:

$$c_L(x) = C_1\, x + C_1 \sqrt{1 - C_2\, x} \tag{70}$$

$$u(x) = C_3\, x + (C_4 - C_5\, x)\sqrt{1 - C_2\, x} - C_4 \tag{71}$$

$$e(x) = C_6 - C_7 \sqrt{1 - C_2\, x} \tag{72}$$

$$\sigma_x = C_8 \tag{73}$$

$$\mathcal{J}_L = C_9 \tag{74}$$

where the C_i, $i \in \{1, ..., 9\}$ are constants that depend on the boundary conditions and material property values. Documentation of the Maple analyses is given in Appendix A.

For the ABAQUS finite element analyses, the 10 $[cm]$ rod is discretized using ten elements of length 1 $[cm]$. The initial concentration and displacement are specified as zero throughout the rod, and the boundary conditions are as indicated in Table 2, and in the figures below. A "coupled temperature-displacement; steady-state" ABAQUS analysis is performed with an initial time increment of 5×10^{-3} $[s]$, a total step time of 1.0 $[s]$, and a maximum allowable increment of 0.5 $[s]$. The residual magnitude for the concentration dof is significantly smaller than the residual for displacement dof. A separate convergence criterion for the concentration (temperature in ABAQUS) dof is therefore adopted. The initial time-average flux for convergence of the concentration dof is set at 5.0×10^{-21} (see the AUM [II;9.6.2-1]). The input decks for the Case 1a and 2a analyses are given in Appendix C.

Case 1a and 2a rod geometries and boundary conditions are shown in Figures 3 and 4. Figures 5 through 11 show plots of: $c_L(x)$; the difference between the linear concentration distribution that obtains from classical SAD and diffusion analysis and $c_L(x)$; $e(x)$; $u(x)$; and $\sigma_x(x)$. Keep in mind while examining these plots that $e(x)$, $\epsilon_x(x)$, $u(x)$, and $\sigma_x(x)$ are identically zero for the classical SAD or diffusion analyses.

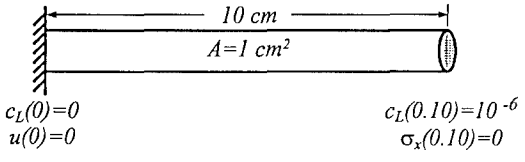


Figure 3: The rod geometry and boundary conditions for Case 1a.

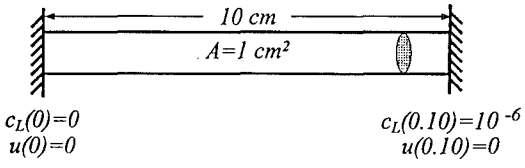


Figure 4: The rod geometry and boundary conditions for Case 2a.

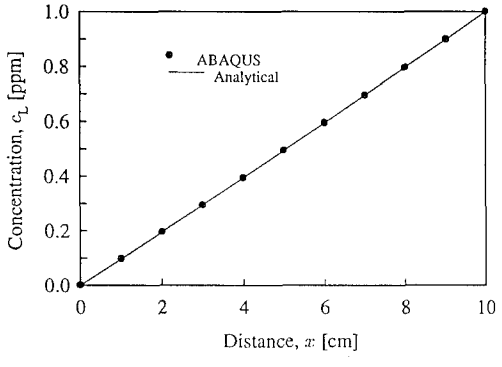


Figure 5: Analytical and finite element concentration predictions for Cases 1a and 2a using the fully coupled theory.

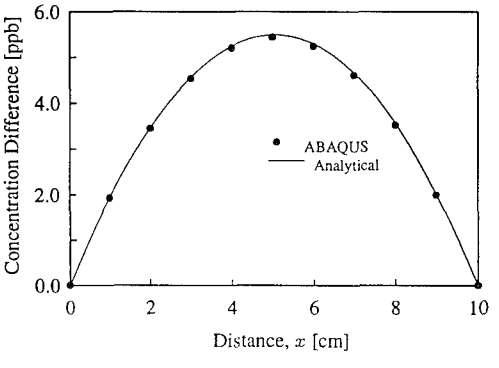


Figure 6: Difference between classical diffusion or SAD and the fully coupled concentrations (i.e., $10^{-7}x - c_L(x)$).

Figures 5 and 6 show the concentration and concentration difference, which are identical for the Case 1a and 2a problems, as a function of position along the rod. The concentration difference is defined as: $10^{-7}x - c_L(x)$ where $10^{-7}x$ is the concentration distribution that obtains for the SAD and classical diffusion theories. The difference is maximum at the center of the rod, but is very small at ≈ 5.5 parts per billion (ppb). The difference between the analytical and finite element predictions is less than 0.05 ppb.

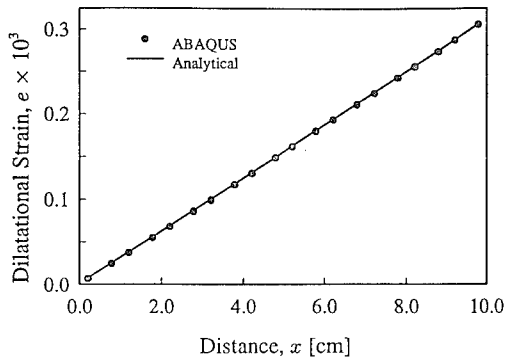


Figure 7: Fully coupled dilatational strain prediction for Case 1a. The FE predictions are given at Gauss integration points.

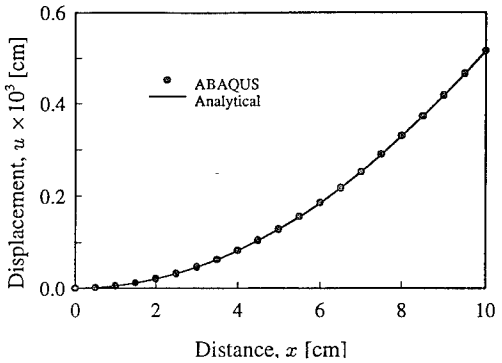


Figure 8: Fully coupled displacement prediction for Case 1a. The FE predictions are given at the nodes.

Figures 7 and 8 show the dilatational strain and the axial displacement experienced by the rod for the case 1a conditions. The rod is traction free, and there are no applied body forces, so by Eq. (18), the stress in the rod must be zero. By way of verification, we note that the FE analysis (not shown) also predicted a zero stress throughout the rod. The maximum dilatational strain and axial displacement occur at the free end of the rod with magnitudes of $\approx 310\,[\mu m/m]$ and $\approx 5.2[\mu m]$ respectively.

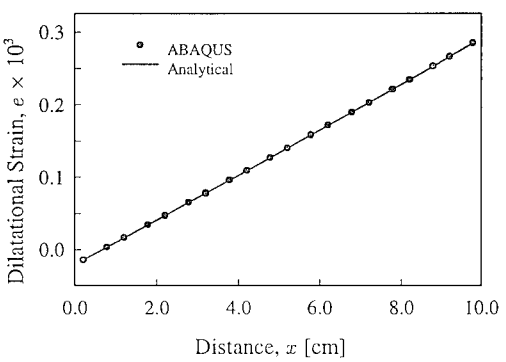


Figure 9: Fully coupled dilatational strain prediction for Case 2a. The FE predictions are given at the Gauss integration points.

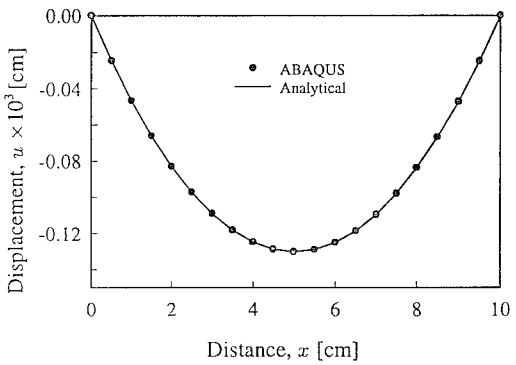


Figure 10: Fully coupled displacement prediction for Case 2a. The FE predictions are given at the nodes.

Figures 9 and 10 show the dilatational strain and axial displacement for Case 2a. The rod, stress free in the absence of hydrogen, tries to expand when the hydrogen is introduced. A uniform axial compressive stress of $\approx 10.4\,[MPa]$ (see Figure 11) is introduced because of the zero displacement boundary restraints at the walls. The dilatational strain is positive and maximum at the RH boundary of the rod, and small, but negative at the LH boundary. The axial displacement is negative throughout the rod indicating a leftward movement of the rod material. The maximum displacement of $\approx -1.3\,[\mu m]$ occurs at the center of the rod. Recalling the definition of axial strain, $\epsilon_x = du/dx$, we see that it is negative in the left half of the bar, positive in the right half, and zero in the middle. The maximum strain ($\approx \pm 50$ $[\mu\epsilon]$) occurs at each end of the rod (see the figure on page A-2a-14 of Appendix A).

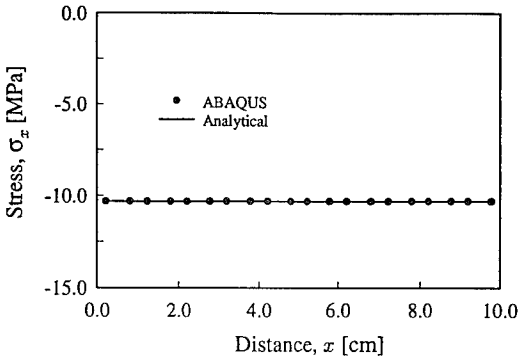


Figure 11: Fully coupled axial stress prediction for Case 2a. The FE predictions are given at the Gauss integration points.

Case 3 Problems

The governing differential equation for the Case 3 problem is obtained from Eq. (66) by substituting in for the applied body force, F_x:

$$\left(1 - \frac{\rho \overline{V}_s^{\,2}\, k}{\mathcal{M}_L \mathbb{R} T}(1 + c_R^s K_R)c_L\right)\frac{dc_L}{dx} + \frac{\overline{V}_s\left(15 \times 10^6\right)}{3\,\mathbb{R} T \sqrt{x^3}}\, c_L = Constant \tag{75}$$

Analytical solutions to this equation are obviously more difficult to obtain than in the previous two cases.

The LHS of Eq. (75) is directly proportional to the mass flux $\mathcal{J}_L$; the mass flux is therefore constant throughout the rod. The Case 3 problem under study imposes a zero mass flux boundary condition on the LH boundary. The constant in Eq. (75) can therefore be set equal to zero, leading to the following governing equation:

$$\left(1 - \frac{\rho \overline{V}_s^{\,2}\, k}{\mathcal{M}_L \mathbb{R} T}(1 + c_R^s K_R)c_L\right)\frac{dc_L}{dx} + \frac{\overline{V}_s\left(15 \times 10^6\right)}{3\,\mathbb{R} T \sqrt{x^3}}\, c_L = 0 \tag{76}$$

This must be solved for c_L as a function of x (i.e., for $c_L(x)$).

An interesting observation regarding Eq. (76) can be made. As $c_L(x)$ increases from some vanishingly small value, the coefficient of the derivative term will go from positive to negative, passing through zero on the way. When the coefficient equals zero, the derivative term drops out and we are left with the equation:

$$\frac{\overline{V}_s\left(15 \times 10^6\right)}{3\,\mathbb{R} T \sqrt{x^3}}\, c_L = 0 \tag{77}$$

This equation cannot be satisfied because c_L is not zero, x is finite-valued, and the rest of the variables are either non-zero constants or material properties. A mathematical solution to the problem can only be obtained by letting $dc_L/dx \to \infty$ as:

$$c_L(x) \rightarrow \frac{\mathcal{M}_L \mathbb{R} T}{\rho \overline{V}_s^2 \, k \, (1 + c_R^s \, K_R)} \tag{78}$$

Allowing this results in multi-valued concentration solutions to Eq. (76); Eq. (78) defines the point at which the solution becomes multi-valued. Since multi-valued concentrations are not physically realistic, the assumptions made in the derivation of the fully coupled transport equations must be re-examined. This is done in the following Discussion section.

The solution to Eq. (76) is obtained by integration using Maple (see Appendix A):

$$c_L(x) = -C_{10} \, W\left(-\frac{exp\left(-C_{11} + \frac{C_{12}}{\sqrt{x}} \right)}{C_{10}} \right) \tag{79}$$

$W(x)$ is Lambert's W function[4], and the C_i, $i \in \{10, 11, 12\}$ are constants related to the material properties and boundary conditions. This equation is multi-valued in x, but it can be inverted to give x as a single-valued function of c_L:

$$x(c_L) = \frac{(C_{12})^2}{\left[\frac{c_L}{C_{10}} - ln(c_L) - C_{11} \right]^2} \tag{80}$$

The stress field is obtained by integrating Eq. (18) with the applied body force substituted in for F_x, yielding:

$$\sigma_x(x) = \frac{30 \times 10^6}{\sqrt{x}} \tag{81}$$

The dilatational strain can be written in terms of σ_x and c_L using Eq. (22b):

$$e(x) = \frac{1}{B_1} (\sigma_x(x) + B_2 \, c_L(x) - B_3) \tag{82}$$

Similar operations can be performed on Eq. (22a) to determine du/dx which can then be integrated (analytical integration may not be possible) to obtain the displacement, $u(x)$.

The ABAQUS analysis for Case 3 requires significantly smaller elements than the Case 1 and 2 analyses, particularly near the singularity. The rod is discretized into 200 elements of length $l_i = 0.104/0.94^{i-1}$ $[\mu m]$ where the first and smallest element, $l_1 = 0.104$ $[\mu m]$, is placed at the left hand end of the bar, $x = 4 \times 10^{-3} [cm]$. The 0.94 factor in the denominator is known as the element "bias" in ABAQUS. A "coupled temperature-displacement; steady-state" analysis is used with an initial time increment of 1.0×10^{-4} $[s]$, a total time of $1.0\,[s]$, and a maximum time increment of 5.0×10^{-3} $[s]$. The initial displacements in the rod are taken as zero, but an initial uniform concentration equal to the RH boundary concentration of 1×10^{-7} $[g\,H/g\,Fe]$ is assumed. To match this initial condition in the analysis, the RH boundary concentration is applied as a step rather than a

[4] Lambert's W function satisfies the equation: $W(x) \times exp\,(W(x)) = x$. Additional information can be found using the interactive Maple V help program.

ramp function. Providing an initial concentration resulted in a more rapid convergence of the solution to the steady-state values. The residual magnitude for the concentration dof is significantly smaller than the residual for displacement dof. A separate convergence criteria for the concentration (temperature in ABAQUS) dof was therefore adopted. The starting time-average flux for convergence of the concentration dof is set at 5.0×10^{-21} (see the AUM [II;9.6.2-1]). The input deck for the Case 3 analysis is given in Appendix C.

The Case 3 rod geometry and boundary conditions are shown in Figure 12. Figures 13 through 17 show: $c_L(x)$; $ln(c_L(x)) - constant$ which illustrates the different concentration singularities; $e(x)$; $u(x)$; and $\sigma_x(x)$. Plots are given for the fully coupled theory under low and high trapping conditions, for SAD theory, and in many cases, for $F_x = 0$. The finite element results are plotted for every 20th element.

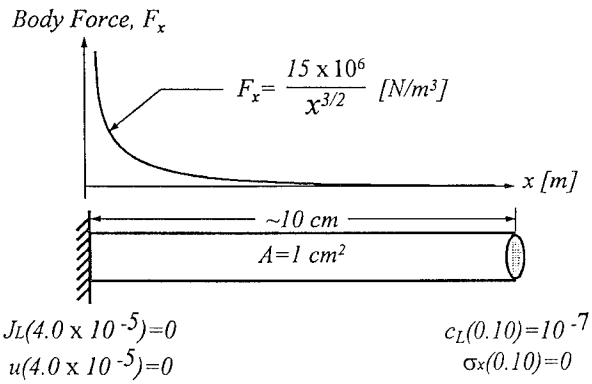


Figure 12: The rod geometry, boundary conditions, and applied body force for the Case 3 problem.

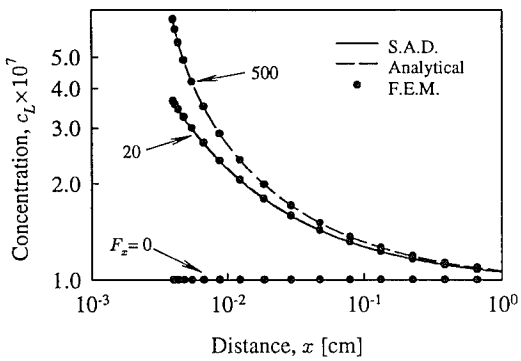


Figure 13: Concentration predictions for Case 3. The SAD results lie under the LT (20) curve of the fully coupled theory.

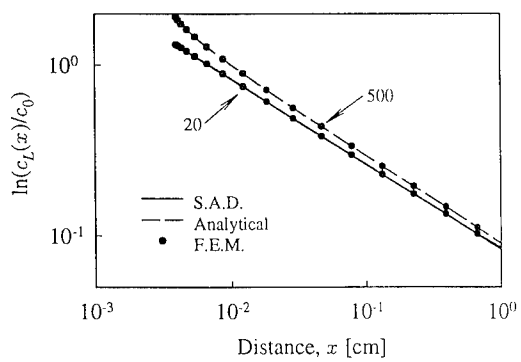


Figure 14: Concentration singularities. The SAD & LT-20 curves are coincident.

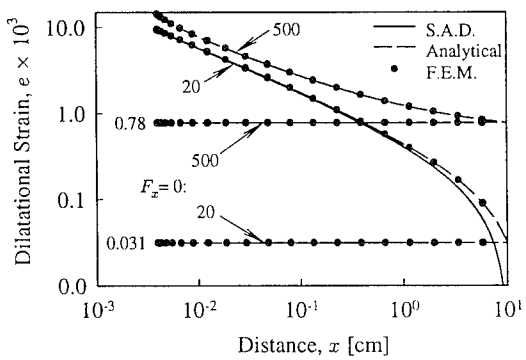


Figure 15: Dilatational strain for Case 3 using the fully coupled and SAD theories.

Figures 13 and 14 show the predicted concentrations for the Case 3 problems using fully coupled and SAD theories. The SAD predictions are made using the classic expression:

$$c_L(x) = c_0 \, exp\left(\frac{\overline{V}_s}{\mathbb{R}T} \times \frac{1}{3} \times \frac{30 \times 10^6}{\sqrt{x}} \right) \tag{83}$$

The fully coupled model predicts slightly larger concentrations than the SAD model, with increasing differences as the singularity is approached and as the degree of trapping increases. Figure 14 shows that the singularity for the fully coupled concentration is more severe than the $exp\left(1/\sqrt{x}\right)$ singularity of the SAD model, at least for the high trapping case.

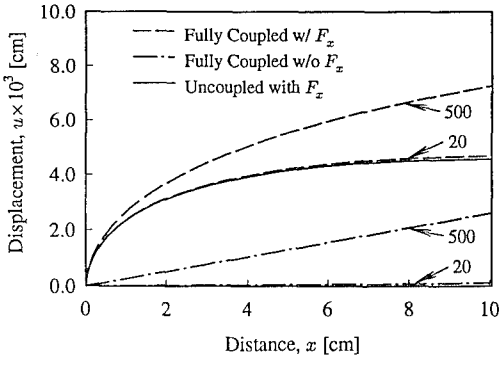


Figure 16: Nodal displacement curves for the FE analysis of Case 3 for the fully coupled and SAD theories.

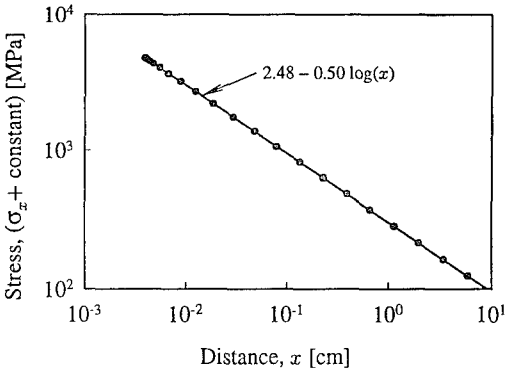


Figure 17: Gauss point stresses with a least squares line fit showing the required straight line behavior with a $-1/2$ slope.

Figures 15 and 16 illustrate the dilatational strains and nodal displacement curves. As with Cases 1 and 2, the fully coupled model predicts larger displacements and dilatational strains throughout the rod. Again, the difference between the fully coupled and SAD model predictions increase with the degree of trapping. The zero-body force strains and displacements are also shown for comparison with the zero valued strains and displacements that obtain for the SAD and classical diffusion model. Figure 17 shows the FE calculated Gauss point stresses; these match the expected behavior.

DISCUSSION

The above three rod problems illustrate the differences between the fully coupled and classical SAD theory under steady-state conditions (additional results can be found in Appendix A). The results show that the concentration differences are generally small, but grow in the region very near to the singularity. The deformation differences are a bit more pronounced, especially in Cases 1 and 2 where the boundary and body force loadings are absent. All of the fully coupled results are dependent on the degree of trapping.

The results also showed that accurate finite element solutions are possible for the fully coupled transport theory using ABAQUS with custom user element subroutines. The experience gained during the development and application of this 1-D user element routine is proving to be very useful in the ongoing development of the 2-D user element subroutine.

The dependence of the concentration and deformation distributions on the trapped hydrogen may be useful in the development of new "Gorsky effect" experiments for trapping characterization. Perhaps the time dependent displacement at the free end of a cantilevered rod can be related to some transport or trapping parameter of interest. Transient Case 1 type problems are probably be most useful in this regard.

Regarding the multi-valued concentrations that appear in the mathematical analysis of the Case 3 problem, the values of c_L satisfying Eq. (78) for the 4340 steel considered are: 2.3×10^{-5} and 9.3×10^{-7} $[g\,H/g\,Fe]$ for the low (LT) and high (HT) trapping conditions, respectively. The *total* internal hydrogen, in mass fraction concentration units[5], is given by Eq. (6): $c_{total} \approx 4.7 \times 10^{-4} + c_I^s$ $[g\,H/g\,Fe]$. Now, this is a very large concentration compared with the solubility of hydrogen in pure iron at room temperature and $1\,[atm]$ pressure ($c_{total} \approx 2 \times 10^{-9}$ $[g\,H/g\,Fe]$ or 1×10^{-7} $[H/Fe]$). It leads us to question the assumptions made regarding the magnitude of the concentration in the development of the fully coupled model. The three major assumptions include: **1.)** "infinite" dilution of the total hydrogen in the mixture; **2.)** ideal behavior; and **3.)** material properties that are independent of the hydrogen concentration level.

The magnitude of the *lattice* concentrations at the critical point are still much less than one. It is unlikely, therefore, that the assumption of infinite dilution is playing any role in this particular situation. Extension of the model to include finite concentrations, while still retaining the ideal solution assumption, can be made by adopting a "reduced" chemical potential [15], which takes into account the blocking of interstitial sites in the neighborhood of a hydrogen atom[6]. Reduced chemical potentials will be adopted in a future version of the theory assuming that the multi-valued solutions for the concentration can be eliminated.

If we maintain the infinite dilution assumption, then non-ideality cannot play a role because an infinitely dilute mixture is by definition, ideal. Non-ideal effects are only possible in finite dilution mixtures [15], and the use of non-ideal expressions in classical SAD modeling is almost non-existent. Kirchheim and Hirth [20] have proposed a first order extension which accounts for H-H interactions. The work by Fukai [21] and coworkers on predicting hydrogen solubility in metals under very high pressures may also be of use in extending our model to include non-ideal effects. The question still remains; will the adoption of a non-ideal chemical potential result in governing equations with single-valued concentrations? We do not presently have an answer for this question; it remains to be investigated in the future.

The last possibility involves the assumption of constant valued material parameters. If the RHS of Eq. (78) were to increase at least linearly with c_L, through some concentration dependence of the material parameters, then the multi-valued solutions will not occur. A linear decrease in ρ, or k, or a square-root decrease in $\overline{V}_s$, with increasing c_L levels would satisfy this requirement. Experimental evidence for these decreases in 4340 steel do not appear to be available in the literature. There is evidence, though, for decreases in $\overline{V}_s$ at large c_L values for various other alloys (see, for example, the article by Peisl in [19; pp. 53-74]; or Fukai [21; pp. 95-100]. This possibility will also have to be investigated in the future.

There remains one final aspect of this multi-valued solution dilemma that needs to be discussed. That is the validity of square-root stress singularities in the fully coupled theory. Remember that this singular body force was artificially introduced in order to get the square-root singular stress. We have not yet determined whether square-root singular stresses will naturally occur at the tip of a crack in the fully coupled theory. The 2-D finite element model under development should shed some light on this issue.

---

[5] Multiplication of c_{total} by $\mathcal{M}_{Fe}/\mathcal{M}_H \approx 55$ gives the mole fraction concentration, $x_{total} = 2.6 \times 10^{-2} + 55\,c_I^s$.

[6] Reduced chemical potentials are also referred to as the "Fermi-Dirac" potentials [20-22].

SUMMARY AND FUTURE RESEARCH

The focus of this research was on the development of a finite element code for coupled hydrogen transport and trapping in linear elastic metals for use in modeling hydrogen assisted cracking processes. A fully coupled solute transport model was developed; a 1-D version of the model was implemented in a finite element code via a custom Fortran "user element" subroutine for use with the ABAQUS finite element program. A series of three simple 1-D problems were posed to develop an understanding of the fully coupled transport theory, and for verifying the accuracy and coding of the 1-D user element subroutine. Steady-state solutions for the fully coupled theory, and for classical diffusion and stress-assisted diffusion theories, were obtained analytically and numerically using the Maple symbolic computation program and ABAQUS. Differences in the predicted concentrations and deformations between the various theories were observed.

One of the problems incorporated a square-root singular stress as a "1-D analog" of the hydrogen transport problem in planar crack geometries. The fully coupled predictions showed slightly higher hydrogen concentrations, a more severe singularity in the concentration, larger axial and dilatational strains, and larger axial displacements, all of which depended on the extent of hydrogen trapping. The results indicated that the hydrogen induced deformations, present only in the fully coupled theory, were more influential with regard to the displacements and strains.

Development of a 2-D user element subroutine is ongoing. The initial versions will be limited in scope to simple linear elastic mixture behavior and equilibrium trapping at reversible and irreversible trap sites. Rectilinear isoparametric 8-node displacement/4-node concentration interpolation functions will be adopted. Extensions of the model to include non-equilibrium trapping effects and plastic crack tip deformations are planned. An effort is also being made to interface the ABAQUS code with our user element routines to the Patran Solid Geometry Modeling program. This will provide us with a convenient means of meshing complex 2-D geometries and manipulating and displaying the finite element results.

After the 2-D code has been developed, it will be used to calculate deformations and concentrations in the crack tip region of a metal with uniform hydrogen concentrations imposed along the crack walls. Steady-state SAD solutions for this idealized problem are available for comparison. The results will provide definitive answers on the importance of the hydrogen induced deformations in crack tip modeling.

A longer term goal is the use of the 2-D code to help establish an energy-based parameter that characterizes the *driving force* for crack growth in the presence of a deleterious environment. This parameter, the *free energy release rate* $\mathcal{F}$, will generalize the classical strain energy release rate $\mathcal{G}$ to include the hydrogen induced deformation energy and the "free" chemical energy. It is defined by:

$$\mathcal{F} := \frac{\Delta(\text{Externally Supplied Work} - \text{Specific Free Energy of the Hydrogen-Metal Mixture})}{\Delta(\text{Crack Length})}$$

The use of $\mathcal{F}$ as a driving force for crack growth in environmentally assisted cracking appears to be a novel extension of the classical fracture mechanics concept. The advantage of $\mathcal{F}$ over the stress intensity factor K (or ΔK) approach will be its ability to account for loading, environment, and material effects on the driving force for crack growth in terms of a single variable. The concept will be applicable many material-environment crack systems of

technological interest including: hydrogen assisted cracking of metals, high temperature oxidation cracking of superalloys, and moisture induced cracking of organic composites.

The magnitude of $\mathcal{F}$ in any environmental cracking situation will have to be determined by an analysis of the deformation and diffusion/trapping processes operative in the crack tip region. More specifically, the deformation state (stresses and strains) and chemical state (potentials and concentrations for each solute species) of the mixture will have to be determined as a function of the loading (e.g., σ or $\Delta\sigma$, R, f, waveform, etc.), environment (e.g., phase, species, concentrations, T, pH, potentials, partial pressures, etc.) and material (e.g., elastic moduli, trapping parameters, solubility, diffusion coefficient, etc.) parameters. This information will be obtained using: **a.)** the fully coupled theory to model the deformation-diffusion-trapping processes occurring in the crack tip region (governing equations); **b.)** an experimentally determined distribution of absorbed species along the crack walls (boundary conditions); and **c.)** a method for solving the resulting mathematical equations (the FE code).

Our initial efforts will be focused on the application of this concept to hydrogen assisted cracking of high strength metals. This system is ideal in the sense that it shows large environmental effects, is important in many applications, and is supported by an extensive data base. It also avoids the complications of large scale crack tip plasticity. Validation of the concept will require demonstration of a unique correlation between the crack growth rate and $\mathcal{F}$ (or $\Delta\mathcal{F}$) for a variety of materials subject to a variety of loading, environment, and material conditions.

ACKNOWLEDGMENTS

The first author's discussions with Dr. Peter Matic of the Naval Research Laboratory concerning various aspects of the theoretical model, and both author's discussions with Dr. David Kirkner of the University of Notre Dame concerning the finite element modeling are gratefully acknowledged. The support of this work by Dr. John Sedriks of the Office of Naval Research under Grant No. N00014-93-1-0845 is also gratefully acknowledged.

REFERENCES

1. J. C. M. Li, R. A. Oriani, and L. S. Darken, (1966), "The Thermodynamics of Stressed Solids", *Z. Physik. Chem.*, Vol. 49, pp. 271-290.
2. H. W. Lui, (1970), "Stress Corrosion Cracking and the Interaction Between Crack-Tip Stress Fields and Solute Atoms", *Trans. ASME-J. Basic Engng.*, Vol. 92, pp. 633-638.
3. P. Sofronis, and R. M. McMeeking, (1989), "Numerical Analysis of Hydrogen Transport Near a Blunting Crack Tip", *J. Mech. Phys. Solids*, Vol. 37, pp. 317-350.
4. H. K. Birnbaum, (1990), "Mechanisms of Hydrogen-Related Fracture of Metals", in *Environment-Induced Cracking of Metals*, Gangloff, R. P., and M. B. Ives, Eds., NACE-10, National Association of Corrosion Engineers, Houston, TX.
5. *Hydrogen Degradation of Ferrous Alloys*, (1985), R. A. Oriani, J. P. Hirth, and M. Smialowski, Eds., Noyes Publications, Park Ridge, NJ.
6. J. P. Hirth, (1980), "Effects of Hydrogen on the Properties of Iron and Steel", *Metall. Trans. A*, Vol. 11A, pp. 861-890.
7. R. N. Iyer and H. W. Pickering, (1990), *Annu. Rev. Mater. Sci.*, Vol. 20, pp. 299-338.
8. A. Turnbull, (1982), "Review of the Electrochemical Conditions in Cracks with Particular Reference to Corrosion Fatigue of Structural Steels in Sea Water", *Reviews in Coatings and Corrosion*, Vol. 5, pp. 43-171.
9. T. R. Beck, (1977), "Techniques for Studying Initial Film Formation on Newly Generated Surfaces of Passive Metals", in *Electrochemical Techniques in Corrosion*, R. Baboian, Nat. Assoc. of Corrosion Engineers, Houston, TX, pp. 27-34.
10. Newman, R. C., (1984), "Measurement and Interpretation of Electrochemical Kinetics on Bare Metal Surfaces" in *Corrosion Chemistry Within Pits, Crevices, and Cracks*, A. Turnbull, Ed., Her Majesty's Stationery Office, London, UK, pp. 317-356.
11. A. McNabb and P. K. Foster, (1963), "A New Analysis of the Diffusion of Hydrogen in Iron and Ferritic Steels", *Trans. TMS-AIME*, Vol. 227, pp. 618-627.
12. B. G. Pound, (1989), "The Application of a Diffusion/Trapping Model for Hydrogen Ingress in High-Strength Alloys", *CORROSION*, Vol. 45, pp. 18-25.
13. H. H. Johnson, (1988), "Hydrogen in Iron", *Metall. Trans. A*, Vol. 19A, pp. 2371-2387.
14. R. Oriani, (1970), "The Diffusion and Trapping of Hydrogen in Steel", *Acta Metall.*,Vol. 18, pp. 147-157.
15. J. P. Thomas, (1993), "A Classical Representation for a Mass based Chemical Potential", *Int. J. Engng. Sci.*, Vol. 31, pp. 1279-1294.
16. K. H. Huebner and E. A. Thorton, (1982), *The Finite Element Method for Engineers*, 2nd ed., Wiley, NY.
17. R. D. Cook, D. S. Malkus, and M. E. Plesha, (1989), *Concepts and Applications of Finite Element Analysis*, 3rd ed., Wiley, NY.
18. *ABAQUS Theory and User's Manuals*, (1993), Standard Version 5.3-1, Hibbitt, Karlson, & Sorensen, Inc., Pawtucket, RI.

19. J. Völkl and G. Alefeld, (1978), "Diffusion of Hydrogen in Metals", in *Hydrogen in Metals I*, Topics in Applied Physics Vol. 28, G. Alefeld and J. Völkl, Eds., Springer, NY, pp. 321-348.
20. R. Kirchheim and J. P. Hirth, (1986), "Hydrogen Absorption at Cracks in Fe, Nb, and Pd", in *Prospectives in Hydrogen in Metals*, M. F. Ashby and J. P. Hirth, Eds., Pergamon Press, NY, pp. 95-98.
21. J. P. Hirth and B. Carnahan, (1978), "Hydrogen Absorption at Dislocations and Cracks", *Acta Metallurgica*, Vol. 26, pp. 1795-1803.
22. Y. Fukai, (1993), *The Metal Hydrogen System*, Springer-Verlag, NY, pp. 53-57 and 95-100.

APPENDIX A: Analytical Solutions Using Maple

This Appendix contains the Maple analyses of the three steady-state rod transport problems studied in this work. All analyses were performed using Maple V, Release 3, on a Sun SPARC 10 workstation. The specific cases analyzed are summarized in the tables below:

Case #	*Deformation Boundary Conditions*		*Diffusion Boundary Conditions*		$c_R^s K_R$	*Page*
1a	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-6}$	19	A-1a-1
1b	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	19	A-1b-1
1c	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	499	A-1c-1
1d	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	19	A-1d-1
1e	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	499	A-1e-1

Table A-1: Case summary for rod problem #1. Displacements, u, are specified in $[m]$; loads, P_x, in $[N]$; concentrations, c_L, in $[kg\,H/kg\,Fe]$; and mass flux, $\mathcal{J}_L$, in $[m/s]$.

Case #	*Deformation Boundary Conditions*		*Diffusion Boundary Conditions*		$c_R^s K_R$	*Page*
2a	$u(LHS) = 0.0$	$u(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-6}$	19	A-2a-1
2b	$u(LHS) = 0.0$	$u(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	19	A-2b-1
2c	$u(LHS) = 0.0$	$u(RHS) = 0.0$	$c_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	499	A-2c-1
2d	$u(LHS) = 0.0$	$u(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	19	A-2d-1
2e	$u(LHS) = 0.0$	$u(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	499	A-2e-1

Table A-2: Summary for rod problem #2. Displacements, u, are specified in $[m]$; concentrations, c_L, in $[kg\,H/kg\,Fe]$; and mass flux, $\mathcal{J}_L$, in $[m/s]$.

Case #	*Deformation Boundary Conditions*		*Diffusion Boundary Conditions*		$c_R^s K_R$	*Body Force*	*Page*
3a	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	19	$\frac{15\times10^6}{\sqrt{x^3}}$	A-3a-1
3a	$u(LHS) = 0.0$	$P_x(RHS) = 0.0$	$\mathcal{J}_L(LHS) = 0.0$	$c_L(RHS) = 10^{-7}$	499	$\frac{15\times10^6}{\sqrt{x^3}}$	A-3a-1

Table A-3: Summary for rod problem #3. The rod length in used in this exact analysis is 10 $[cm]$, in distinction with the rod length used in the finite element analysis. Displacements, u, are specified in $[m]$; loads, P_x, in $[N]$; concentrations, c_L, in $[kg\,H/kg\,Fe]$; mass flux, $\mathcal{J}_L$, in $[m/s]$; and body force, F_x, in $[N/m^3]$.

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#1a.ms

==========

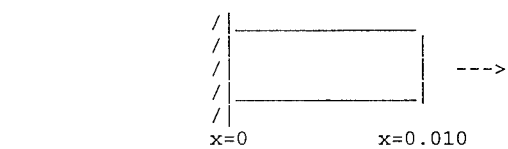
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, S(0.10)=0
Concentration variable boundary conditions: c(0)=0, c(0.10)=1e-6
Reference concentration level: c0=0.0
Trapping parameter: traps=19 (low trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=diff(J,x)=0;

$$deqn := Ds\,K1\,K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)^2 + Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial^2}{\partial x^2}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} - \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2},$$

$$\mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} + \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2}$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         boundary conditions will be used to select the proper one.
```

> c1:=unapply(simplify(op(2,csoln[1])),x);

$$c1 := x \rightarrow \frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c1(x);

$$\frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow -\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2(x);

$$-\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> J1:=unapply(simplify(Ds*(K1*K2*c1(x)-1)*diff(c1(x),x),x));

$$J1 := (\,) \rightarrow Ds\,_C1$$

> J1(x);

$$Ds\,_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := (\,) \rightarrow Ds\,_C1$$

> J2(x);

$$Ds\,_C1$$

Note #2: The above results show that both mass flux solutions are identical
and equal to Ds*_C1 where _C1 is a constant of integration!

> ex1:=dsolve(diff(e(x),x)-K2*diff(c1(x),x)=0,e(x));

$$ex1 := \mathrm{e}(x) = \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1:=unapply(simplify(op(2,ex1)),x);

$$e1 := x \rightarrow \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1(x);

$$\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> ex2:=dsolve(diff(e(x),x)-K2*diff(c2(x),x)=0,e(x));

$$ex2 := \mathrm{e}(x) = \frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e2:=unapply(simplify(op(2,ex2)),x);

$$e2 := x \rightarrow \frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e2(x);

$$\frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

```
> ux1:=dsolve(A1*diff(u(x),x)+A2*c1(x)-A3-e1(x)=0,u(x));
```

$$ux1 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> u1:=unapply(simplify(op(2,ux1)),x);
```

$$u1 := x \to \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2 + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,x + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

```
> u1(x);
```

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));
```

$$ux2 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> u2:=unapply(simplify(op(2,ux2)),x);
```

$$u2 := x \to \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\right.$$

$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,x$$
$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,_C2+3\,A3\,x\,K1^2\,K2^2\,_C1$$
$$-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,x$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,_C2+3\,_C3\,x\,K1^2\,K2^2\,_C1$$
$$+3\,_C4\,A1\,K1^2\,K2^2\,_C1\Big)\Big/(A1\,K1^2\,K2^2\,_C1)$$

```
> u2(x);
```

$$\frac{1}{3}\Big(-3\,A2\,x\,K1\,K2\,_C1+A2\sqrt{\%1}+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,x+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,_C2$$
$$+3\,A3\,x\,K1^2\,K2^2\,_C1-\sqrt{\%1}\;K2-2\sqrt{\%1}\;K2^2\,K1\,_C1\,x-2\sqrt{\%1}\;K2^2\,K1\,_C1\,_C2$$
$$+3\,_C3\,x\,K1^2\,K2^2\,_C1+3\,_C4\,A1\,K1^2\,K2^2\,_C1\Big)\Big/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2$$

```
> S1:=x->simplify(B1*e1(x)-B2*c1(x)+B3);
```

$$S1 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e1}(x)-B2\;\mathrm{c1}(x)+B3)$$

```
> S1(x);
```

$$\Big(B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B1\,K2\,_C3\,K1-B2$$
$$-B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B3\,K1\,K2\Big)\Big/(K1\,K2)$$

```
> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);
```

$$S2 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e2}(x)-B2\;\mathrm{c2}(x)+B3)$$

```
> S2(x);
```

$$\Big(-B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B1\,K2\,_C3\,K1-B2$$
$$+B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B3\,K1\,K2\Big)\Big/(K1\,K2)$$

```
Note #3: At this point, we will introduce expressions for the constants and
         then simplify the results before quantifying the constants and
         determining the constants of integration.
```

```
> K:=(Em/(3*(1-2*nu)));
```

$$K := \frac{Em}{3-6\,\nu}$$

```
> lambda:=(Em*nu)/((1+nu)*(1-2*nu));
```

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2+2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\frac{\rho\, Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\, Em}{(3 - 6\,\nu)\, R\, T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\, Vs\, (1 + traps)}{MWs}$$

```
> K1*K2;
```

$$\frac{Vs^2\, Em\, \rho\, (1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)\, c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\,\frac{Em\, \rho\, Vs\, (1 + traps)}{(3 - 6\,\nu)\, MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\,\frac{Em\, \rho\, Vs\, (1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c1(x);

$$\left(1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> c2(x);

$$-\left(-1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> e1(x);

$$\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> e2(x);

$$\left(-\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> u1(x);

$$\frac{1}{3}\left(-2\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}-\frac{2}{3}\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$
$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$+2\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}+\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$
$$+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$\left.+3\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}\right)$$
$$(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\left((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\right)$$

$$\%1 := 1 + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, x}{(3-6\,\nu)\, R\, T\, MWs} + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, _C2}{(3-6\,\nu)\, R\, T\, MWs}$$

```
> u2(x);
```

$$\frac{1}{3}\left(-2\frac{(1+\nu)\,\rho^2\, Vs^3\,(1+traps)^2\, x\, Em\, _C1}{MWs^2\,(3-6\,\nu)\, R\, T} + \frac{2}{3}\frac{(1+\nu)\,\rho\, Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$

$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, x}{MWs^2\,(3-6\,\nu)\, R\, T}$$

$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, _C2}{MWs^2\,(3-6\,\nu)\, R\, T}$$

$$+2\frac{(1+\nu)\,\rho^3\, Vs^5\,(1+traps)^3\, c0\, x\, Em^2\, _C1}{MWs^3\,(3-6\,\nu)^2\, R^2\, T^2} - \frac{\sqrt{\%1}\,\rho\, Vs\,(1+traps)}{MWs}$$

$$-2\frac{\sqrt{\%1}\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, x}{MWs^2\,(3-6\,\nu)\, R\, T} - 2\frac{\sqrt{\%1}\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, _C2}{MWs^2\,(3-6\,\nu)\, R\, T}$$

$$+3\frac{_C3\, x\, Vs^4\, Em^2\, \rho^2\,(1+traps)^2\, _C1}{(3-6\,\nu)^2\, R^2\, T^2\, MWs^2} + 3\frac{_C4\,(1-2\,\nu)\, Vs^4\, Em^2\, \rho^2\,(1+traps)^2\, _C1}{(3-6\,\nu)^2\, R^2\, T^2\, MWs^2}$$

$$\left.\right)(3-6\,\nu)^2\, R^2\, T^2\, MWs^2 \Big/ \left((1-2\,\nu)\, Vs^4\, Em^2\, \rho^2\,(1+traps)^2\, _C1\right)$$

$$\%1 := 1 + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, x}{(3-6\,\nu)\, R\, T\, MWs} + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, _C2}{(3-6\,\nu)\, R\, T\, MWs}$$

```
> S1(x);
```

$$-(MWs\, _C3\, Vs\, Em - 3\, R\, T\, MWs + 6\, R\, T\, MWs\, \nu + Em\, \rho\, Vs^2\, c0 + Em\, \rho\, Vs^2\, c0\, traps) \Big/ ((-1+2\,\nu)\, Vs\, MWs)$$

```
> S2(x);
```

$$-(MWs\, _C3\, Vs\, Em - 3\, R\, T\, MWs + 6\, R\, T\, MWs\, \nu + Em\, \rho\, Vs^2\, c0 + Em\, \rho\, Vs^2\, c0\, traps) \Big/ ((-1+2\,\nu)\, Vs\, MWs)$$

```
> S1(x)-S2(x);
```

$$0$$

```
Note #4: The stresses are same for each solution root, and do not depend on
         the position x! The stresses are therefore constant throughout the
         body. We will solve for _C3 in terms of the boundary stress, S0.
```

```
> _C3:=simplify(solve(S1(x)=S0,_C3));
```

$$_C3 := -(-3\, R\, T\, MWs + 6\, R\, T\, MWs\, \nu + Em\, \rho\, Vs^2\, c0 + Em\, \rho\, Vs^2\, c0\, traps - S0\, Vs\, MWs + 2\, S0\, Vs\, MWs\, \nu) \Big/ (MWs\, Vs\, Em)$$

> S1(x);

$$S0$$

> S2(x);

$$S0$$

> S1:=x->S0;

$$S1 := x \rightarrow S0$$

> S2:=x->S0;

$$S2 := x \rightarrow S0$$

```
Note #5: Now we will introduce numerical values for the material properties.
         The values selected are typical for internal hydrogen as a
         solute in AISI 4340 steel.
```

> S0:=0.0;

$$S0 := 0$$

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=19;

$$traps := 19$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$312.628352034286$$

> K1*K2;

$$43205.0114421104$$

> 1/(K1*K2);

$$.0000231454631447068$$

> A1;

$$.4$$

> A2;

$$270.944571763048$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.156314176017143\ 10^{15}$$

> B3;

$$0$$

> _C3;

$$.00723592800000000$$

> S1(x);

$$0$$

> S2(x);

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, and _C4, using the boundary data.

> c1(x);

$$\frac{.0000231454631447068 + .0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> c2(x);

$$\frac{.0000231454631447068 - .0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> evalf(c1(x),5);

$$.000023146 + .000023146\sqrt{1. + 86408.\ _C1\ x + 86408.\ _C1\ _C2}$$

```
> eqnset1:={0=c1(0),1e-6=c1(0.10)};
```

$$eqnset1 := \left\{ .1\ 10^{-5} = .0000231454631447068 + .0000231454631447068 \sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}, 0 = .0000231454631447068 + .0000231454631447068 \sqrt{1 + 86410.0228842208\ _C1\ _C2} \right\}$$

```
> varset1:={_C1,_C2};
```

$$varset1 := \{ _C2, _C1 \}$$

```
> solnset1:=solve(eqnset1,varset1);
```

$$solnset1 :=$$

```
> eqnset2:={0=c2(0),1e-6=c2(0.10)};
```

$$eqnset2 := \left\{ .1\ 10^{-5} = .0000231454631447068 - .0000231454631447068 \sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}, 0 = .0000231454631447068 - .0000231454631447068 \sqrt{1 + 86410.0228842208\ _C1\ _C2} \right\}$$

```
> varset2:={_C1,_C2};
```

$$varset2 := \{ _C2, _C1 \}$$

```
> solnset2:=solve(eqnset2,varset2);
```

$$solnset2 := \{ _C1 = -.978397494278943\ 10^{-5}, _C2 = 0 \}$$

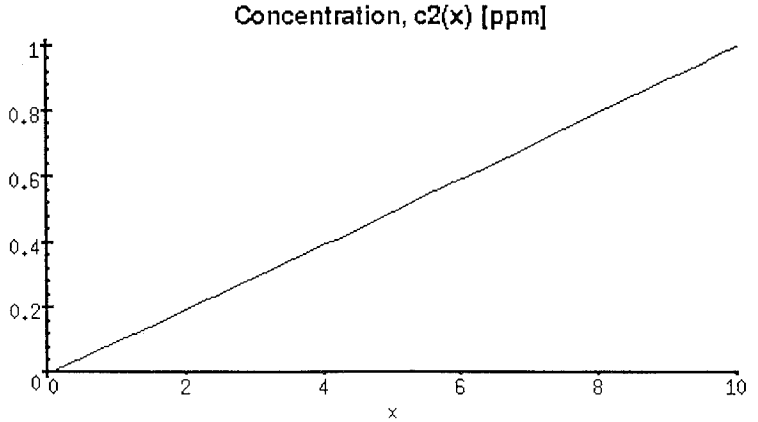
```
> assign(solnset2);
```

```
Note #7: The solution c1(x) is not capable of satisfying the boundary
         conditions, as evidenced by the lack of solution for the given
         boundary conditions. The concentration function c2(x) is the
         correct solution in this case!
```

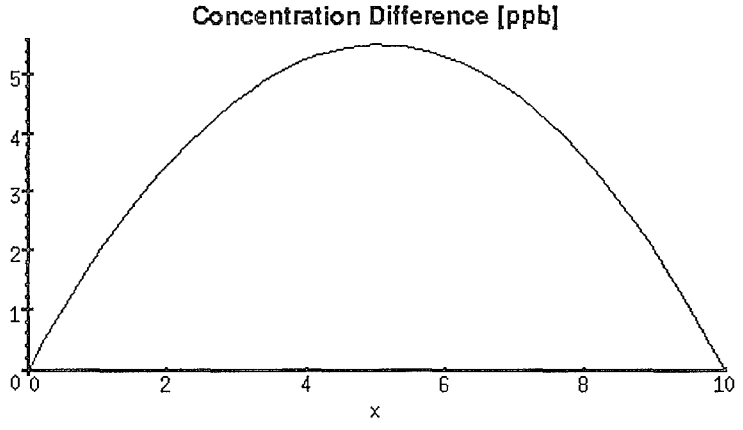
```
> c2(x);
```

$$.0000231454631447068 - .0000231454631447068 \sqrt{1 - .845433498705078\ x}$$

```
> p1:=plot(1e6*c2(x/100),x=0..10,title='Concentration, c2(x) [ppm]'):
> p1;
>
```



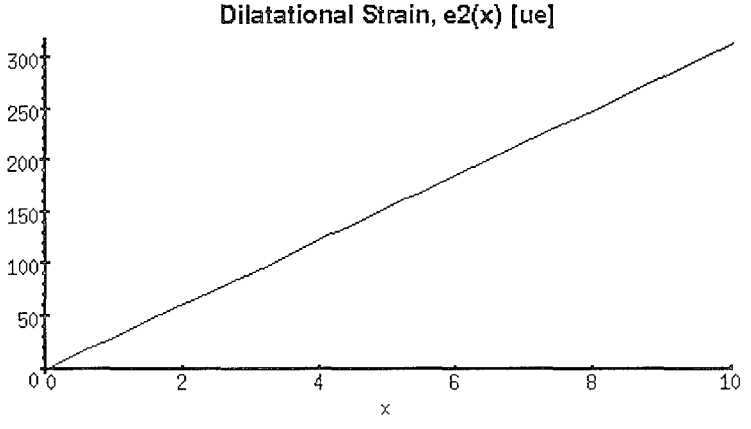
```
> p2:=plot(1e9*(c2(0)+((c2(0.10)-c2(0))/0.10)*x/100-c2(x/100)),x=0..10,title='Concentration Difference [ppb]'):
> p2;
>
```



```
> e2(x);
```

$$-.00723592799999998\sqrt{1 - .845433498705078\,x} + .00723592799999998$$

```
> p3:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p3;
>
```



```
> u2(x);
```

$$.00241197600000008\,x + .00190196390663828\sqrt{1 - .845433498705078\,x}$$
$$- .00160798400000005\sqrt{1 - .845433498705078\,x}\,x + .999999999999996\,_C4$$

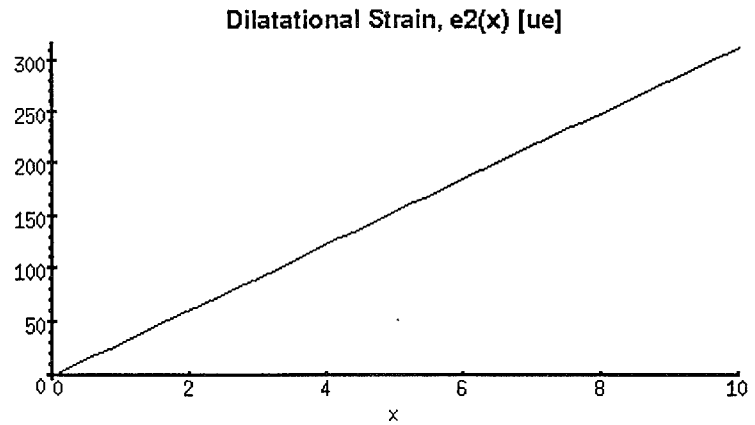
```
> _C4:=solve(u2(0)=0,_C4);
```

$$_C4 := -.00190196390663829$$

```
> u2(x);
```

$$.00241197600000008\,x + .00190196390663828\sqrt{1 - .845433498705078\,x}$$
$$- .00160798400000005\sqrt{1 - .845433498705078\,x}\,x - .00190196390663827$$

```
> p4:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p4;
>
```



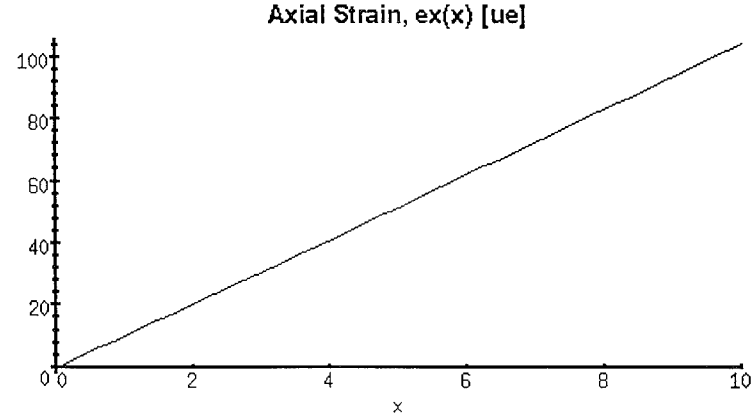
```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := x \rightarrow .00241197600000008 - .000803991999999990 \frac{1}{\sqrt{1 - .845433498705078\, x}} + .000679721769490914 \frac{x}{\sqrt{1 - .845433498705078\, x}} - .00160798400000005 \sqrt{1 - .845433498705078\, x}$$

```
> ex(x);
```

$$.00241197600000008 - .000803991999999990 \frac{1}{\sqrt{1 - .845433498705078\, x}} + .000679721769490914 \frac{x}{\sqrt{1 - .845433498705078\, x}} - .00160798400000005 \sqrt{1 - .845433498705078\, x}$$

```
> p5:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p5;
>
```



```
> evalf(u2(x),5);
```

$$.0024108\,x + .0019015\sqrt{1. - .84542\,x} - .0016072\sqrt{1. - .84542\,x}\,x - .0019021$$

```
> evalf(c2(x),5);
```

$$.000023146 - .000023146\sqrt{1. - .84542\,x}$$

```
> evalf(e2(x),5);
```

$$-.0072359\sqrt{1. - .84542\,x} + .0072359$$

```
> evalf(ex(x),5);
```

$$.0024120 - .00080399\frac{1}{\sqrt{1. - .84543\,x}} + .00067972\frac{x}{\sqrt{1. - .84543\,x}} - .0016080\sqrt{1. - .84543\,x}$$

```
> J2(x);
```

$$-.978397494278943\ 10^{-14}$$

```
>
```

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#1b.ms

==========

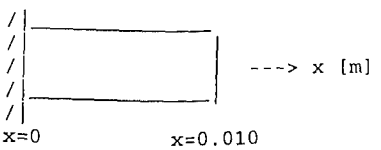
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, S(0.10)=0
Concentration variable boundary conditions: c(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=19 (low trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

=====================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

=====================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=diff(J,x)=0;

$$deqn := Ds\,K1\,K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)^2 + Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial^2}{\partial x^2}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} - \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2},$$

$$\mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} + \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2}$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         boundary conditions will be used to select the proper one.
```

> c1:=unapply(simplify(op(2,csoln[1])),x);

$$c1 := x \rightarrow \frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c1(x);

$$\frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow -\frac{-1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2(x);

$$-\frac{-1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> J1:=unapply(simplify(Ds*(K1*K2*c1(x)-1)*diff(c1(x),x),x));

$$J1 := (\,) \rightarrow Ds\,_C1$$

> J1(x);

$$Ds\,_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := (\,) \rightarrow Ds\,_C1$$

> J2(x);

$$Ds\,_C1$$

Note #2: The above results show that both mass flux solutions are identical and equal to Ds*_C1 where _C1 is a constant of integration!

> ex1:=dsolve(diff(e(x),x)-K2*diff(c1(x),x)=0,e(x));

$$ex1 := \mathrm{e}(x) = \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> e1:=unapply(simplify(op(2,ex1)),x);

$$e1 := x \rightarrow \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> e1(x);

$$\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> ex2:=dsolve(diff(e(x),x)-K2*diff(c2(x),x)=0,e(x));

$$ex2 := \mathrm{e}(x) = \frac{-\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> e2:=unapply(simplify(op(2,ex2)),x);

$$e2 := x \rightarrow -\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - _C3\,K1}{K1}$$

> e2(x);

$$-\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - _C3\,K1}{K1}$$

```
> ux1:=dsolve(A1*diff(u(x),x)+A2*c1(x)-A3-e1(x)=0,u(x));
```

$$ux1 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> u1:=unapply(simplify(op(2,ux1)),x);
```

$$u1 := x \rightarrow -\frac{1}{3}\left(3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,_C2 - 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2 - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,x - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,_C2 - 3\,_C3\,x\,K1^2\,K2^2\,_C1 - 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

```
> u1(x);
```

$$-\frac{1}{3}\left(3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 - 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 - 3\,_C3\,x\,K1^2\,K2^2\,_C1 - 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));
```

$$ux2 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> u2:=unapply(simplify(op(2,ux2)),x);
```

$$u2 := x \rightarrow \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\right.$$

$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,x$$
$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,_C2+3\,A3\,x\,K1^2\,K2^2\,_C1$$
$$-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,x$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,_C2+3\,_C3\,x\,K1^2\,K2^2\,_C1$$
$$+3\,_C4\,A1\,K1^2\,K2^2\,_C1\Big)\Big/(A1\,K1^2\,K2^2\,_C1)$$

> u2(x);

$$\frac{1}{3}\Big(-3\,A2\,x\,K1\,K2\,_C1+A2\sqrt{\%1}+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,x+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,_C2$$
$$+3\,A3\,x\,K1^2\,K2^2\,_C1-\sqrt{\%1}\;K2-2\sqrt{\%1}\;K2^2\,K1\,_C1\,x-2\sqrt{\%1}\;K2^2\,K1\,_C1\,_C2$$
$$+3\,_C3\,x\,K1^2\,K2^2\,_C1+3\,_C4\,A1\,K1^2\,K2^2\,_C1\Big)\Big/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2$$

> S1:=x->simplify(B1*e1(x)-B2*c1(x)+B3);

$$S1 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e1}(x)-B2\;\mathrm{c1}(x)+B3)$$

> S1(x);

$$\Big(B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B1\,K2\,_C3\,K1-B2$$
$$-B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B3\,K1\,K2\Big)\Big/(K1\,K2)$$

> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);

$$S2 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e2}(x)-B2\;\mathrm{c2}(x)+B3)$$

> S2(x);

$$\Big(-B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B1\,K2\,_C3\,K1-B2$$
$$+B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B3\,K1\,K2\Big)\Big/(K1\,K2)$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

> K:=(Em/(3*(1-2*nu)));

$$K := \frac{Em}{3-6\,\nu}$$

> lambda:=(Em*nu)/((1+nu)*(1-2*nu));

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

> mu:=Em/(2*(1+nu));

$$\mu := \frac{Em}{2+2\,\nu}$$

> alpha:=(rho*Vs)/(3*MWs);

$$\alpha := \frac{1}{3}\frac{\rho\, Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\, Em}{(3 - 6\,\nu)\, R\, T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\, Vs\,(1 + traps)}{MWs}$$

```
> K1*K2;
```

$$\frac{Vs^2\, Em\, \rho\,(1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)\, c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\frac{Em\,\rho\, Vs\,(1 + traps)}{(3 - 6\,\nu)\, MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\frac{Em\,\rho\, Vs\,(1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c1(x);

$$\left(1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> c2(x);

$$-\left(-1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> e1(x);

$$\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> e2(x);

$$-\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}-\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> u1(x);

$$-\frac{1}{3}\left(2\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}+\frac{2}{3}\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$
$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$-2\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}-\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$
$$-2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}-2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$\left.-3\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}-3\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}\right)$$
$$(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\left((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\right)$$

$$\%1 := 1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}$$

> u2(x);

$$\frac{1}{3}\left(-2\,\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em_C1}{MWs^2\,(3-6\,\nu)\,R\,T}+\frac{2}{3}\,\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\,\sqrt{\%1}}{MWs}\right.$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+2\,\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}-\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$

$$-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+3\,\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\,\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}$$

$$\left.\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\Big((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\Big)$$

$$\%1 := 1+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1_C2}{(3-6\,\nu)\,R\,T\,MWs}$$

> S1(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/((-1+2\,\nu)\,Vs\,MWs)$$

> S2(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/((-1+2\,\nu)\,Vs\,MWs)$$

> S1(x)-S2(x);

$$0$$

```
Note #4: The stresses are same for each solution root, and do not depend on
         the position x! The stresses are therefore constant throughout the
         body. We will solve for _C3 in terms of the boundary stress, S0.
```

> _C3:=simplify(solve(S1(x)=S0,_C3));

$$_C3 := -(-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps-S0\,Vs\,MWs+2\,S0\,Vs\,MWs\,\nu)\Big/(Em\,MWs\,Vs)$$

> S1(x);

$$S0$$

> S2(x);

$$S0$$

```
> S1:=x->S0;
```

$$S1 := x \rightarrow S0$$

```
> S2:=x->S0;
```

$$S2 := x \rightarrow S0$$

```
Note #5: Now we will introduce numerical values for the material properties.
         The values selected are typical for internal hydrogen as a
         solute in AISI 4340 steel.
```

```
> S0:=0.0;
```

$$S0 := 0$$

```
> Ds:=1e-9;
```

$$Ds := .1\ 10^{-8}$$

```
> Vs:=2.02e-6;
```

$$Vs := .202\ 10^{-5}$$

```
> traps:=19;
```

$$traps := 19$$

```
> c0:=0.0;
```

$$c0 := 0$$

```
> MWs:=0.00100797;
```

$$MWs := .00100797$$

```
> Em:=200e9;
```

$$Em := .200\ 10^{12}$$

```
> nu:=0.3;
```

$$\nu := .3$$

```
> rho:=7800;
```

$$\rho := 7800$$

```
> T:=293;
```

$$T := 293$$

```
> R:=8.31432;
```

$$R := 8.31432$$

```
> K;
```

$$.166666666666667\ 10^{12}$$

```
> lambda;
```

$$.115384615384616\ 10^{12}$$

```
> mu;
```

$$.769230769230769\ 10^{11}$$

```
> alpha;
```

$$5.21047253390476$$

```
> Rh:=R/MWs;
```

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$312.628352034286$$

> K1*K2;

$$43205.0114421104$$

> 1/(K1*K2);

$$.0000231454631447068$$

> A1;

$$.4$$

> A2;

$$270.944571763048$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.156314176017143\ 10^{15}$$

> B3;

$$0$$

> _C3;

$$.00723592800000000$$

> S1(x);

$$0$$

> S2(x);

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, and _C4, using the boundary data.

> c1(x);

$$\frac{.0000231454631447068 + .0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> c2(x);

$$\frac{.0000231454631447068 - .0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> evalf(c1(x),5);

$$.000023146 + .000023146\sqrt{1. + 86408.\ _C1\ x + 86408.\ _C1\ _C2}$$

> eqnset1:={0=c1(0),1e-7=c1(0.10)};

$$eqnset1 := \{0 = .0000231454631447068 + .0000231454631447068\sqrt{1 + 86410.0228842208\ _C1\ _C2},\ .1\ 10^{-6} = .0000231454631447068 + .0000231454631447068\sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}\}$$

```
> varset1:={_C1,_C2};
```

$$varset1 := \{_C1, _C2\}$$

```
> solnset1:=solve(eqnset1,varset1);
```

$$solnset1 :=$$

```
> eqnset2:={0=c2(0),1e-7=c2(0.10)};
```

$$eqnset2 := \{0 = .0000231454631447068 - .0000231454631447068\sqrt{1 + 86410.0228842208\ _C1\ _C2},\ .1\ 10^{-6} = .0000231454631447068 - .0000231454631447068\sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}\}$$

```
> varset2:={_C1,_C2};
```

$$varset2 := \{_C1, _C2\}$$

```
> solnset2:=solve(eqnset2,varset2);
```

$$solnset2 := \{_C1 = -.997839749427893\ 10^{-6}, _C2 = 0\}$$

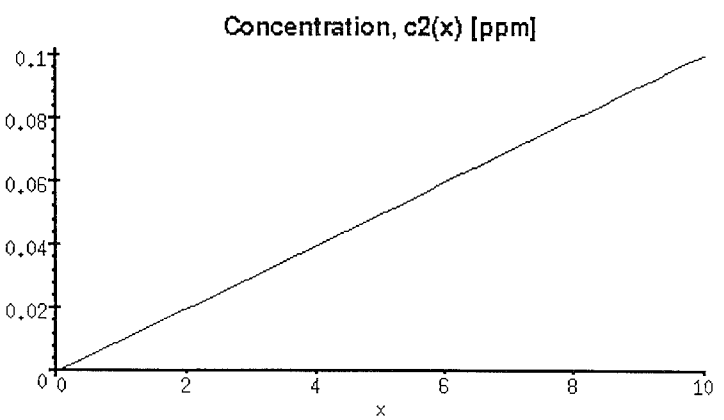
```
> assign(solnset2);
```

```
Note #7: The solution c1(x) is not capable of satisfying the boundary
         conditions, as evidenced by the lack of solution for the given
         boundary conditions. The concentration function c2(x) is the
         correct solution in this case!
```

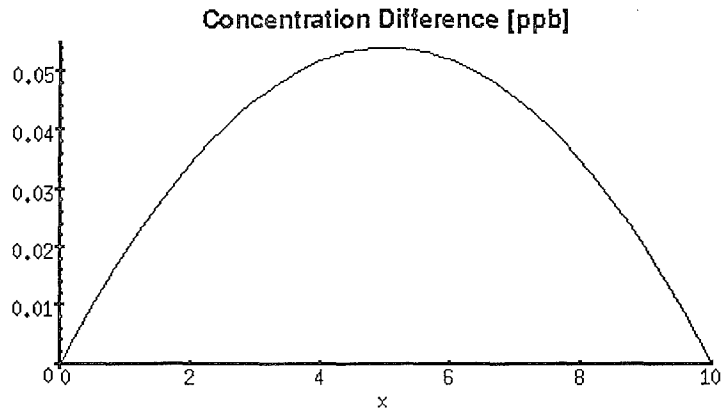
```
> c2(x);
```

$$.0000231454631447068 - .0000231454631447068\sqrt{1 - .0862233555828494\ x}$$

```
> p1:=plot(1e6*c2(x/100),x=0..10,title='Concentration, c2(x) [ppm]'):
> p1;
>
```



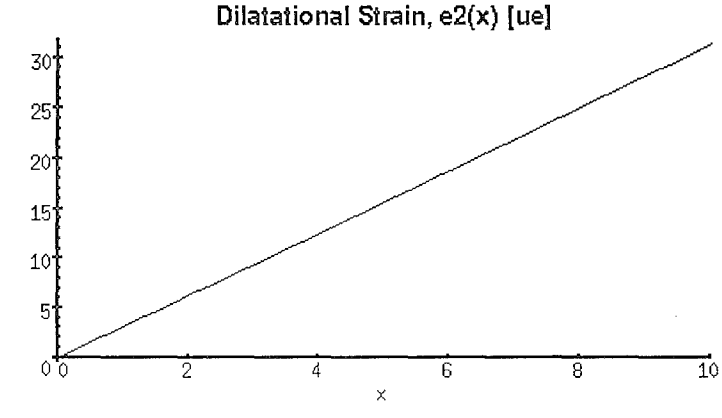
```
> p2:=plot(1e9*(c2(0)+((c2(0.10)-c2(0))/0.10)*x/100-c2(x/100)),x=0..10,title='Concentration Difference [ppb]'):
> p2;
>
```



```
> e2(x);
```

$$-.00723592799999998\sqrt{1 - .0862233555828494\,x} + .00723592799999998$$

```
> p3:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p3;
>
```



```
> u2(x);
```

$$.00241197600000003\,x + .0186490538338527\sqrt{1 - .0862233555828494\,x}$$
$$- .00160798400000002\sqrt{1 - .0862233555828494\,x}\,x + .999999999999992\,_C4$$

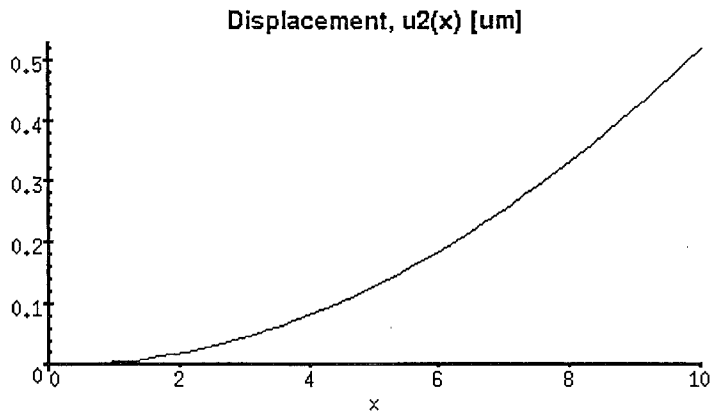
```
> _C4:=solve(u2(0)=0,_C4);
```

$$_C4 := -.0186490538338528$$

```
> u2(x);
```

$$.00241197600000003\,x + .0186490538338527\sqrt{1 - .0862233555828494\,x}$$
$$- .00160798400000002\sqrt{1 - .0862233555828494\,x}\,x - .0186490538338526$$

```
> p4:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p4;
>
```



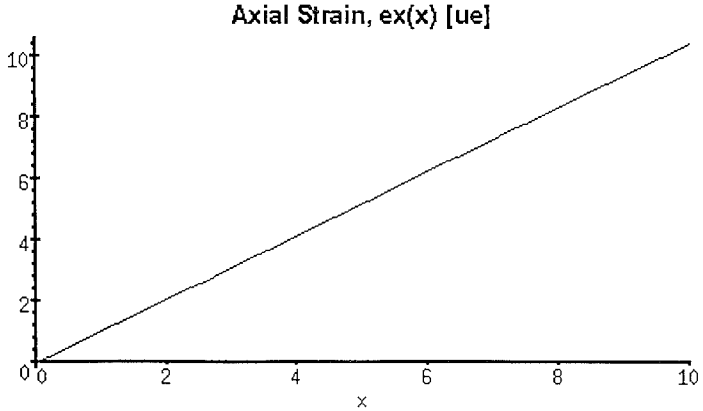
```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := x \rightarrow .00241197600000003 - .000803991999999991 \frac{1}{\sqrt{1 - .0862233555828494\,x}} + .000069322888101767 1 \frac{x}{\sqrt{1 - .0862233555828494\,x}} - .00160798400000002 \sqrt{1 - .0862233555828494\,x}$$

```
> ex(x);
```

$$.00241197600000003 - .000803991999999991 \frac{1}{\sqrt{1 - .0862233555828494\,x}} + .000069322888101767 1 \frac{x}{\sqrt{1 - .0862233555828494\,x}} - .00160798400000002 \sqrt{1 - .0862233555828494\,x}$$

```
> p5:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p5;
>
```



> evalf(u2(x),5);

$$.0024107\,x + .018644\sqrt{1. - .086222\,x} - .0016072\sqrt{1. - .086222\,x}\,x - .018650$$

> evalf(c2(x),5);

$$.000023146 - .000023146\sqrt{1. - .086222\,x}$$

> evalf(e2(x),5);

$$-.0072359\sqrt{1. - .086222\,x} + .0072359$$

> evalf(ex(x),5);

$$.0024120 - .00080399\frac{1}{\sqrt{1. - .086223\,x}} + .000069323\frac{x}{\sqrt{1. - .086223\,x}} - .0016080\sqrt{1. - .086223\,x}$$

> J2(x);

$$-.997839749427893\ 10^{-15}$$

---

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#1c.ms

==========

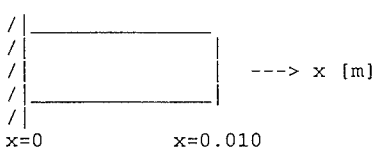
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: 21-Jan-1995
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, S(0.10)=0
Concentration variable boundary conditions: c(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=499 (high trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=diff(J,x)=0;

$$deqn := Ds\,K1\,K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)^2 + Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial^2}{\partial x^2}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} - \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2},$$

$$\mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} + \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2}$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         boundary conditions will be used to select the proper one.
```

> c1:=unapply(simplify(op(2,csoln[1])),x);

$$c1 := x \rightarrow \frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c1(x);

$$\frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow -\frac{-1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2(x);

$$-\frac{-1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> J1:=unapply(simplify(Ds*(K1*K2*c1(x)-1)*diff(c1(x),x),x));

$$J1 := (\,) \rightarrow Ds\,_C1$$

> J1(x);

$$Ds\,_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := (\,) \rightarrow Ds\,_C1$$

> J2(x);

$$Ds\,_C1$$

```
Note #2: The above results show that both mass flux solutions are identical
         and equal to Ds*_C1 where _C1 is a constant of integration!
```

> ex1:=dsolve(diff(e(x),x)-K2*diff(c1(x),x)=0,e(x));

$$ex1 := \mathrm{e}(x) = \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> e1:=unapply(simplify(op(2,ex1)),x);

$$e1 := x \rightarrow \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> e1(x);

$$\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + _C3\,K1}{K1}$$

> ex2:=dsolve(diff(e(x),x)-K2*diff(c2(x),x)=0,e(x));

$$ex2 := \mathrm{e}(x) = -\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - _C3\,K1}{K1}$$

> e2:=unapply(simplify(op(2,ex2)),x);

$$e2 := x \rightarrow -\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - _C3\,K1}{K1}$$

> e2(x);

$$-\frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - _C3\,K1}{K1}$$

> ux1:=dsolve(A1*diff(u(x),x)+A2*c1(x)-A3-e1(x)=0,u(x));

$$ux1 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> u1:=unapply(simplify(op(2,ux1)),x);

$$u1 := x \to \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2 + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,x + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

> u1(x);

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));

$$ux2 := \mathrm{u}(x) = -\frac{1}{3}\left(3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 - 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 - 3\,_C3\,x\,K1^2\,K2^2\,_C1 - 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> u2:=unapply(simplify(op(2,ux2)),x);

$$u2 := x \to \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\right.$$

$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,x$$
$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,_C2+3\,A3\,x\,K1^2\,K2^2\,_C1$$
$$-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,x$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,_C2+3\,_C3\,x\,K1^2\,K2^2\,_C1$$
$$+3\,_C4\,A1\,K1^2\,K2^2\,_C1\Big)\Big/(A1\,K1^2\,K2^2\,_C1)$$

```
> u2(x);
```

$$\frac{1}{3}\Big(-3\,A2\,x\,K1\,K2\,_C1+A2\sqrt{\%1}+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,x+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,_C2$$
$$+3\,A3\,x\,K1^2\,K2^2\,_C1-\sqrt{\%1}\;K2-2\sqrt{\%1}\;K2^2\,K1\,_C1\,x-2\sqrt{\%1}\;K2^2\,K1\,_C1\,_C2$$
$$+3\,_C3\,x\,K1^2\,K2^2\,_C1+3\,_C4\,A1\,K1^2\,K2^2\,_C1\Big)\Big/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2$$

```
> S1:=x->simplify(B1*e1(x)-B2*c1(x)+B3);
```

$$S1 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e1}(x)-B2\;\mathrm{c1}(x)+B3)$$

```
> S1(x);
```

$$\Big(B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B1\,K2\,_C3\,K1-B2$$
$$-B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B3\,K1\,K2\Big)\Big/(K1\,K2)$$

```
> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);
```

$$S2 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e2}(x)-B2\;\mathrm{c2}(x)+B3)$$

```
> S2(x);
```

$$-\Big(B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-B1\,K2\,_C3\,K1+B2$$
$$-B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-B3\,K1\,K2\Big)\Big/(K1\,K2)$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

```
> K:=(Em/(3*(1-2*nu)));
```

$$K := \frac{Em}{3-6\,\nu}$$

```
> lambda:=(Em*nu)/((1+nu)*(1-2*nu));
```

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2+2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\frac{\rho\, Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\, Em}{(3 - 6\,\nu)\, R\, T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\, Vs\,(1 + traps)}{MWs}$$

```
> K1*K2;
```

$$\frac{Vs^2\, Em\, \rho\,(1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)\, c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)}{(3 - 6\,\nu)\, MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c1(x);

$$\left(1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T\,MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> c2(x);

$$-\left(-1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T\,MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> e1(x);

$$\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> e2(x);

$$-\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}-\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> u1(x);

$$\frac{1}{3}\left(-2\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}-\frac{2}{3}\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\,\sqrt{\%1}}{MWs}\right.$$

$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+2\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}+\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$

$$+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$\left.+3\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\left((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\right)$$

$$\%1 := 1 + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, x}{(3-6\,\nu)\, R\, T\, MWs} + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, _C2}{(3-6\,\nu)\, R\, T\, MWs}$$

```
> u2(x);
```

$$\frac{1}{3}\left(-2\frac{(1+\nu)\,\rho^2\, Vs^3\,(1+traps)^2\, x\, Em\, _C1}{MWs^2\,(3-6\,\nu)\, R\, T} + \frac{2}{3}\frac{(1+\nu)\,\rho\, Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$

$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, x}{MWs^2\,(3-6\,\nu)\, R\, T}$$

$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, _C2}{MWs^2\,(3-6\,\nu)\, R\, T}$$

$$+2\frac{(1+\nu)\,\rho^3\, Vs^5\,(1+traps)^3\, c0\, x\, Em^2\, _C1}{MWs^3\,(3-6\,\nu)^2\, R^2\, T^2} - \frac{\sqrt{\%1}\,\rho\, Vs\,(1+traps)}{MWs}$$

$$-2\frac{\sqrt{\%1}\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, x}{MWs^2\,(3-6\,\nu)\, R\, T} - 2\frac{\sqrt{\%1}\,\rho^2\, Vs^3\,(1+traps)^2\, Em\, _C1\, _C2}{MWs^2\,(3-6\,\nu)\, R\, T}$$

$$+3\frac{_C3\, x\, Vs^4\, Em^2\, \rho^2\,(1+traps)^2\, _C1}{(3-6\,\nu)^2\, R^2\, T^2\, MWs^2} + 3\frac{_C4\,(1-2\,\nu)\, Vs^4\, Em^2\, \rho^2\,(1+traps)^2\, _C1}{(3-6\,\nu)^2\, R^2\, T^2\, MWs^2}$$

$$\left.\right)(3-6\,\nu)^2\, R^2\, T^2\, MWs^2 \Big/ \left((1-2\,\nu)\, Vs^4\, Em^2\, \rho^2\,(1+traps)^2\, _C1\right)$$

$$\%1 := 1 + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, x}{(3-6\,\nu)\, R\, T\, MWs} + 2\frac{Vs^2\, Em\, \rho\, (1+traps)\, _C1\, _C2}{(3-6\,\nu)\, R\, T\, MWs}$$

```
> S1(x);
```

$$-(MWs\, _C3\, Vs\, Em - 3\, R\, T\, MWs + 6\, R\, T\, MWs\, \nu + Em\, \rho\, Vs^2\, c0 + Em\, \rho\, Vs^2\, c0\, traps) \Big/ ((-1+2\,\nu)\, Vs\, MWs)$$

```
> S2(x);
```

$$-(MWs\, _C3\, Vs\, Em - 3\, R\, T\, MWs + 6\, R\, T\, MWs\, \nu + Em\, \rho\, Vs^2\, c0 + Em\, \rho\, Vs^2\, c0\, traps) \Big/ ((-1+2\,\nu)\, Vs\, MWs)$$

```
> S1(x)-S2(x);
```

$$0$$

```
Note #4: The stresses are same for each solution root, and do not depend on
         the position x! The stresses are therefore constant throughout the
         body. We will solve for _C3 in terms of the boundary stress, S0.
```

```
> _C3:=simplify(solve(S1(x)=S0,_C3));
```

$$_C3 := -(-3\, R\, T\, MWs + 6\, R\, T\, MWs\, \nu + Em\, \rho\, Vs^2\, c0 + Em\, \rho\, Vs^2\, c0\, traps - S0\, Vs\, MWs + 2\, S0\, Vs\, MWs\, \nu) \Big/ (Em\, Vs\, MWs)$$

> S1(x);

$$S0$$

> S2(x);

$$S0$$

> S1:=x->S0;

$$S1 := x \rightarrow S0$$

> S2:=x->S0;

$$S2 := x \rightarrow S0$$

Note #5: Now we will introduce numerical values for the material properties.
The values selected are typical for internal hydrogen as a
solute in AISI 4340 steel.

> S0:=0.0;

$$S0 := 0$$

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=499;

$$traps := 499$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$7815.70880085715$$

> K1*K2;

$$.108012528605276\ 10^{7}$$

> 1/(K1*K2);

$$.925818525788271\ 10^{-6}$$

> A1;

$$.4$$

> A2;

$$6773.61429407620$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.390785440042860\ 10^{16}$$

> B3;

$$0$$

> _C3;

$$.00723592800000000$$

> S1(x);

$$0$$

> S2(x);

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, and _C4, using the boundary data.

> c1(x);

$$\frac{.925818525788271\ 10^{-6} + .925818525788271\ 10^{-6}}{\sqrt{1 + .216025057210552\ 10^{7}\ _C1\ x + .216025057210552\ 10^{7}\ _C1\ _C2}}$$

> c2(x);

$$\frac{.925818525788271\ 10^{-6} - .925818525788271\ 10^{-6}}{\sqrt{1 + .216025057210552\ 10^{7}\ _C1\ x + .216025057210552\ 10^{7}\ _C1\ _C2}}$$

> evalf(c1(x),5);

$$.92584\ 10^{-6} + .92584\ 10^{-6}\sqrt{1. + .21602\ 10^{7}\ _C1\ x + .21602\ 10^{7}\ _C1\ _C2}$$

```
> eqnset1:={0=c1(0),1e-7=c1(0.10)};
```

$$eqnset1 := \{ .1\ 10^{-6} = .925818525788271\ 10^{-6} + .925818525788271\ 10^{-6} \sqrt{1 + 216025.057210552\ _C1 + .216025057210552\ 10^{7}\ _C1\ _C2}, 0 = .925818525788271\ 10^{-6} + .925818525788271\ 10^{-6}\sqrt{1 + .216025057210552\ 10^{7}\ _C1\ _C2} \}$$

```
> varset1:={_C1,_C2};
```

$$varset1 := \{ _C1, _C2 \}$$

```
> solnset1:=solve(eqnset1,varset1);
```

$$solnset1 :=$$

```
> eqnset2:={0=c2(0),1e-7=c2(0.10)};
```

$$eqnset2 := \{ 0 = .925818525788271\ 10^{-6} - .925818525788271\ 10^{-6}\sqrt{1 + .216025057210552\ 10^{7}\ _C1\ _C2}, .1\ 10^{-6} = .925818525788271\ 10^{-6} - .925818525788271\ 10^{-6} \sqrt{1 + 216025.057210552\ _C1 + .216025057210552\ 10^{7}\ _C1\ _C2} \}$$

```
> varset2:={_C1,_C2};
```

$$varset2 := \{ _C1, _C2 \}$$

```
> solnset2:=solve(eqnset2,varset2);
```

$$solnset2 := \{ _C1 = -.945993735697361\ 10^{-6}, _C2 = 0 \}$$

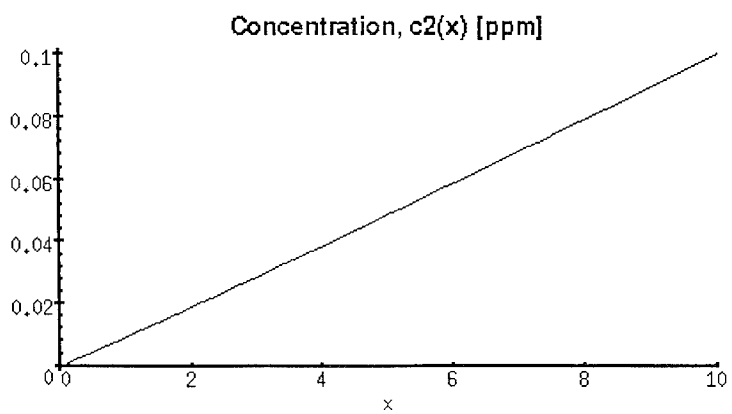
```
> assign(solnset2);
```

```
  Note #7: The solution c1(x) is not capable of satisfying the boundary
           conditions, as evidenced by the lack of solution for the given
           boundary conditions. The concentration function c2(x) is the
           correct solution in this case!
```

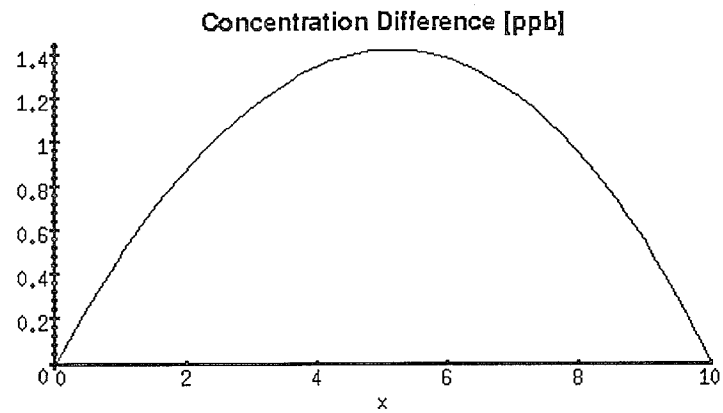
```
> c2(x);
```

$$.925818525788271\ 10^{-6} - .925818525788271\ 10^{-6}\sqrt{1 - 2.04358350874846\ x}$$

```
> p1:=plot(1e6*c2(x/100),x=0..10,title='Concentration, c2(x) [ppm]'):
> p1;
>
```



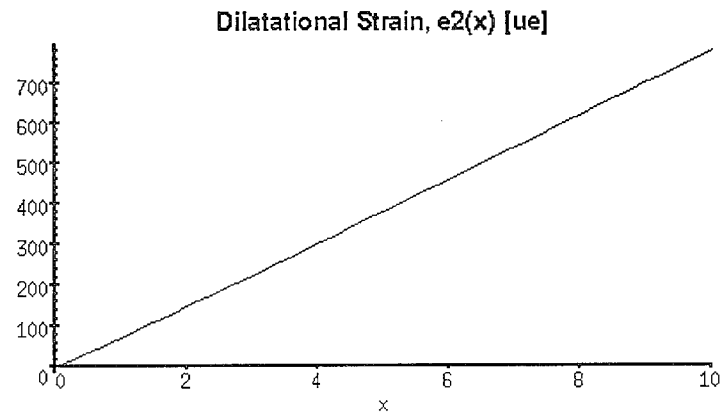
```
> p2:=plot(1e9*(c2(0)+((c2(0.10)-c2(0))/0.10)*x/100-c2(x/100)),x=0..10,title='Concentration Difference [ppb]'):
> p2;
>
```



```
> e2(x);
```

$$-.00723592799999998\sqrt{1 - 2.04358350874846\,x} + .00723592799999998$$

```
> p3:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p3;
>
```



```
> u2(x);
```

$$.00241197599999993\,x + .000786845261334466\sqrt{1 - 2.04358350874846\,x}$$
$$- .00160798399999998\sqrt{1 - 2.04358350874846\,x}\,x + .999999999999996\,_C4$$

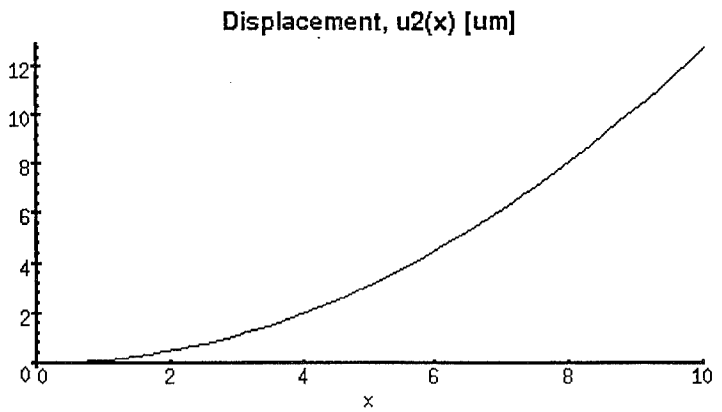
```
> _C4:=solve(u2(0)=0,_C4);
```

$$_C4 := -.000786845261334469$$

```
> u2(x);
```

$$.00241197599999993\,x + .000786845261334466\sqrt{1 - 2.04358350874846\,x}$$
$$- .00160798399999998\sqrt{1 - 2.04358350874846\,x}\,x - .000786845261334466$$

```
> p4:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p4;
>
```



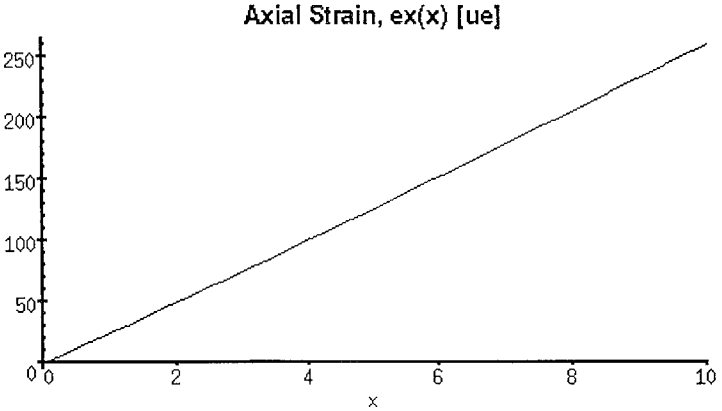
```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := x \rightarrow .00241197599999993 - .000803991999999993 \frac{1}{\sqrt{1 - 2.04358350874846\,x}} + .00164302479236567 \frac{x}{\sqrt{1 - 2.04358350874846\,x}} - .00160798399999998 \sqrt{1 - 2.04358350874846\,x}$$

```
> ex(x);
```

$$.00241197599999993 - .000803991999999993 \frac{1}{\sqrt{1 - 2.04358350874846\,x}} + .00164302479236567 \frac{x}{\sqrt{1 - 2.04358350874846\,x}} - .00160798399999998 \sqrt{1 - 2.04358350874846\,x}$$

```
> p5:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p5;
>
```



```
> evalf(u2(x),5);
```

$$.0024118\,x + .00078643\sqrt{1. - 2.0436\,x} - .0016069\sqrt{1. - 2.0436\,x}\,x - .00078689$$

```
> evalf(c2(x),5);
```

$$.92584\,10^{-6} - .92584\,10^{-6}\sqrt{1. - 2.0436\,x}$$

```
> evalf(e2(x),5);
```

$$-.0072359\sqrt{1. - 2.0436\,x} + .0072366$$

```
> evalf(ex(x),5);
```

$$.0024120 - .00080399\frac{1}{\sqrt{1. - 2.0436\,x}} + .0016430\frac{x}{\sqrt{1. - 2.0436\,x}} - .0016080\sqrt{1. - 2.0436\,x}$$

```
> J2(x);
```

$$-.945993735697361\,10^{-15}$$

---

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#1d.ms

==========

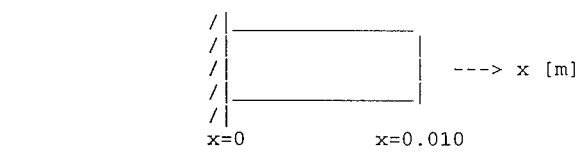
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, S(0.10)=0
Concentration variable boundary conditions: J(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=19 (low trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

=====================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

=====================

6. SYMBOLIC ANALYSIS:
```

```
> restart;
> Digits:=trunc(evalhf(Digits));
```

$$Digits := 15$$

```
> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);
```

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

```
> deqn:=J=0;
```

$$deqn := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) = 0$$

```
> csoln:=dsolve(deqn,c(x),explicit);
```

$$csoln := \mathrm{c}(x) = \frac{1}{K1\,K2},\ \mathrm{c}(x) = _C1$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         first solution is obviously incorrect in that the concentration
         throughout the rod is defined in terms of the constants K1 and K2.
         The second solution is adopted as correct.
```

```
> c2:=unapply(simplify(op(2,csoln[2])),x);
```

$$c2 := x \rightarrow _C1$$

```
> c2(x);
```

$$_C1$$

```
> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));
```

$$J2 := 0$$

```
> J2(x);
```

$$0$$

```
Note #2: The above results show that the mass flux is identically zero, as
         it should be.
```

> e2:=x->_C2;

$$e2 := x \rightarrow _C2$$

> e2(x);

$$_C2$$

> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));

$$ux2 := \mathrm{u}(x) = \frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

> u2:=unapply(simplify(op(2,ux2)),x);

$$u2 := x \rightarrow \frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

> u2(x);

$$\frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);

$$S2 := x \rightarrow \mathrm{simplify}(B1\ \mathrm{e2}(x) - B2\ \mathrm{c2}(x) + B3)$$

> S2(x);

$$B1\ _C2 - B2\ _C1 + B3$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

> K:=(Em/(3*(1-2*nu)));

$$K := \frac{Em}{3 - 6\,\nu}$$

> lambda:=(Em*nu)/((1+nu)*(1-2*nu));

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

> mu:=Em/(2*(1+nu));

$$\mu := \frac{Em}{2 + 2\,\nu}$$

> alpha:=(rho*Vs)/(3*MWs);

$$\alpha := \frac{1}{3}\,\frac{\rho\ Vs}{MWs}$$

> K1:=(Vs*K)/(R*T);

$$K1 := \frac{Vs\ Em}{(3 - 6\,\nu)\,R\,T}$$

> K2:=3*alpha*(1+traps);

$$K2 := \frac{\rho\, Vs\,(1 + traps)}{MWs}$$

> K1*K2;

$$\frac{Vs^2\, Em\, \rho\,(1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

> A1:=(1-2*nu);

$$A1 := 1 - 2\,\nu$$

> A2:=2*(1+nu)*alpha*(1+traps);

$$A2 := \frac{2}{3}\,\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)}{MWs}$$

> A3:=A2*c0;

$$A3 := \frac{2}{3}\,\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)\, c0}{MWs}$$

> B1:=3*K;

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

> B2:=9*K*alpha*(1+traps);

$$B2 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)}{(3 - 6\,\nu)\, MWs}$$

> B3:=B2*c0;

$$B3 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c2(x);

$$_C1$$

> e2(x);

$$_C2$$

> u2(x);

$$\left(-\frac{2}{3}\,\frac{x\,(1 + \nu)\,\rho\, Vs\,(1 + traps)\,_C1}{MWs} + \frac{2}{3}\,\frac{x\,(1 + \nu)\,\rho\, Vs\,(1 + traps)\, c0}{MWs} + x\,_C2 + _C3\,(1 - 2\,\nu)\right) \Big/ (1 - 2\,\nu)$$

> S2(x);

$$\frac{Em\,(-_C2\, MWs + \rho\, Vs\,_C1 + \rho\, Vs\,_C1\, traps - \rho\, Vs\, c0 - \rho\, Vs\, c0\, traps)}{(-1 + 2\,\nu)\, MWs}$$

Note #4: Now we will introduce numerical values for the material properties.
The values selected are typical for internal hydrogen as a
solute in AISI 4340 steel.

> S0:=0.0;

$$S0 := 0$$

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=19;

$$traps := 19$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31696;

$$R := 8.31696$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8251.19795232001$$

> K1;

$$138.155406787625$$

> K2;

$$312.628352034286$$

> K1*K2;

$$43191.2971486416$$

```
> 1/(K1*K2);
```

$$.0000231528123954816$$

```
> A1;
```

$$.4$$

```
> A2;
```

$$270.944571763048$$

```
> A3;
```

$$0$$

```
> B1;
```

$$.500000000000001\ 10^{12}$$

```
> B2;
```

$$.156314176017143\ 10^{15}$$

```
> B3;
```

$$0$$

```
  Note #6: Now let's solve for the integration constants: _C1, _C2, and _C3, using the
           boundary data.
```

```
> c2(x);
```

$$_C1$$

```
> _C1:=1e-7;
```

$$_C1 := .1\ 10^{-6}$$

```
> c2(x);
```

$$.1\ 10^{-6}$$

```
> u2(x);
```

$$-.0000677361429407620\ x + 2.50000000000000\ x\ _C2 + 1.00000000000000\ _C3$$

```
> S2(x);
```

$$.500000000000001\ 10^{12}\ _C2 - .156314176017143\ 10^{8}$$

```
> _C2:=solve(S2(0.1)=0.0,_C2);
```

$$_C2 := .0000312628352034285$$

```
> S2(x);
```

$$0$$

```
> u2(x);
```

$$.0000104209450678093\ x + 1.00000000000000\ _C3$$

```
> _C3:=solve(u2(0.0)=0,_C3);
```

$$_C3 := 0$$

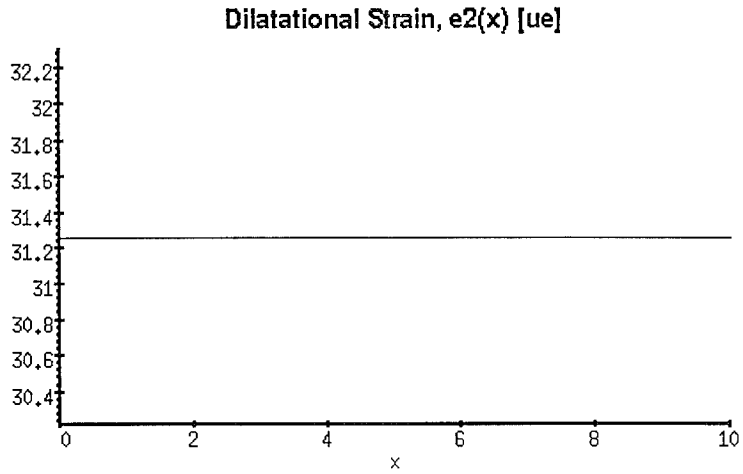
```
> u2(x);
```

$$.0000104209450678093\ x$$

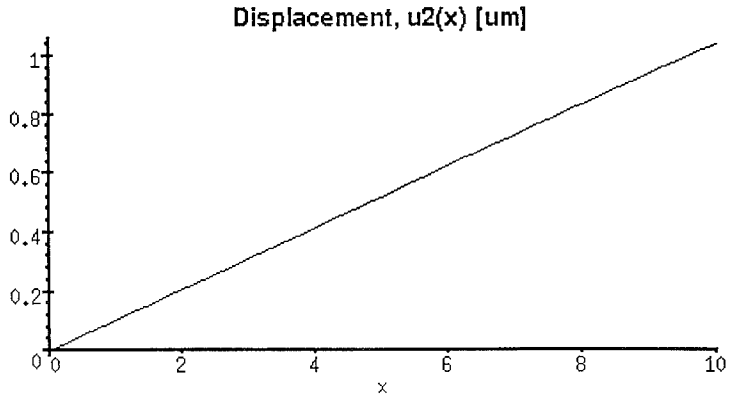
```
> e2(x);
```

.0000312628352034285

```
> p1:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p1;
>
```



```
> p2:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p2;
>
```



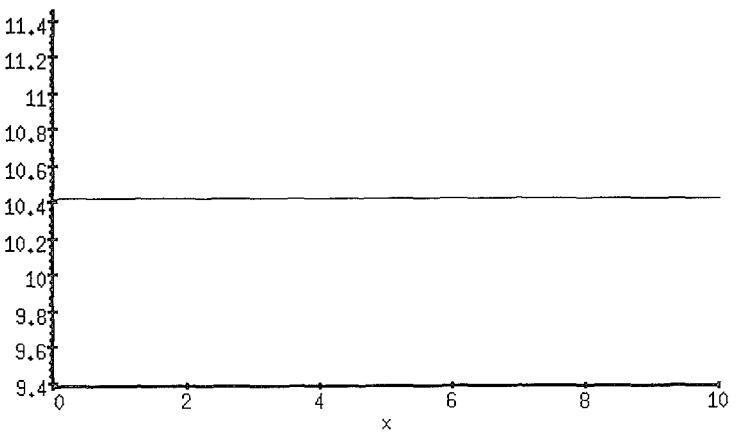
```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := .0000104209450678093$$

```
> ex(x);
```

$$.0000104209450678093$$

```
> p3:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p3;
>
```



```
> evalf(10^6*u2(x),5);
```

$$10.420\,x$$

```
> evalf(c2(x),5);
```

$$.1\ 10^{-6}$$

```
> evalf(10^6*e2(x),5);
```

$$31.263$$

```
> evalf(10^6*ex(x),5);
```

$$10.421$$

---

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#1e.ms

==========

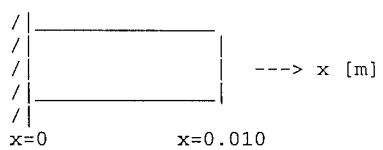
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, S(0.10)=0
Concentration variable boundary conditions: J(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=499 (high trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

=====================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

=====================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=J=0;

$$deqn := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = \frac{1}{K1\,K2},\ \mathrm{c}(x) = _C1$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         first solution is obviously incorrect in that the concentration
         throughout the rod is defined in terms of the constants K1 and K2.
         The second solution is adopted as correct.
```

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow _C1$$

> c2(x);

$$_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := 0$$

> J2(x);

$$0$$

```
Note #2: The above results show that the mass flux is identically zero, as
         it should be.
```

> e2:=x->_C2;

$$e2 := x \rightarrow _C2$$

> e2(x);

$$_C2$$

> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));

$$ux2 := \mathrm{u}(x) = -\frac{x\,A2\,_C1 - x\,A3 - x\,_C2 - _C3\,A1}{A1}$$

> u2:=unapply(simplify(op(2,ux2)),x);

$$u2 := x \rightarrow -\frac{x\,A2\,_C1 - x\,A3 - x\,_C2 - _C3\,A1}{A1}$$

> u2(x);

$$-\frac{x\,A2\,_C1 - x\,A3 - x\,_C2 - _C3\,A1}{A1}$$

> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);

$$S2 := x \rightarrow \mathrm{simplify}(B1\ \mathrm{e2}(x) - B2\ \mathrm{c2}(x) + B3)$$

> S2(x);

$$B1\ _C2 - B2\ _C1 + B3$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

> K:=(Em/(3*(1-2*nu)));

$$K := \frac{Em}{3 - 6\,\nu}$$

> lambda:=(Em*nu)/((1+nu)*(1-2*nu));

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

> mu:=Em/(2*(1+nu));

$$\mu := \frac{Em}{2 + 2\,\nu}$$

> alpha:=(rho*Vs)/(3*MWs);

$$\alpha := \frac{1}{3}\frac{\rho\,Vs}{MWs}$$

> K1:=(Vs*K)/(R*T);

$$K1 := \frac{Vs\,Em}{(3 - 6\,\nu)\,R\,T}$$

> K2:=3*alpha*(1+traps);

$$K2 := \frac{\rho\ Vs\ (1 + traps)}{MWs}$$

> K1*K2;

$$\frac{Vs^2\ Em\ \rho\ (1 + traps)}{(3 - 6\ \nu)\ R\ T\ MWs}$$

> A1:=(1-2*nu);

$$A1 := 1 - 2\ \nu$$

> A2:=2*(1+nu)*alpha*(1+traps);

$$A2 := \frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)}{MWs}$$

> A3:=A2*c0;

$$A3 := \frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ c0}{MWs}$$

> B1:=3*K;

$$B1 := 3\ \frac{Em}{3 - 6\ \nu}$$

> B2:=9*K*alpha*(1+traps);

$$B2 := 3\ \frac{Em\ \rho\ Vs\ (1 + traps)}{(3 - 6\ \nu)\ MWs}$$

> B3:=B2*c0;

$$B3 := 3\ \frac{Em\ \rho\ Vs\ (1 + traps)\ c0}{(3 - 6\ \nu)\ MWs}$$

> c2(x);

$$_C1$$

> e2(x);

$$_C2$$

> collect(u2(x),x);

$$-\frac{\left(\frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ _C1}{MWs} - \frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ c0}{MWs} - _C2\right) x}{1 - 2\ \nu} + _C3$$

> S2(x);

$$\frac{Em\ (-_C2\ MWs + \rho\ Vs\ _C1 + \rho\ Vs\ _C1\ traps - \rho\ Vs\ c0 - \rho\ Vs\ c0\ traps)}{(-1 + 2\ \nu)\ MWs}$$

Note #4: Now we will introduce numerical values for the material properties.
The values selected are typical for internal hydrogen as a
solute in AISI 4340 steel.

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=499;

$$traps := 499$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$7815.70880085715$$

> K1*K2;

$$.108012528605276\ 10^{7}$$

> 1/(K1*K2);

$$.925818525788271\ 10^{-6}$$

> A1;

$$.4$$

> A2;

$$6773.61429407620$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.390785440042860\ 10^{16}$$

> B3;

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, and _C3, using the boundary data.

> c2(x);

$$_C1$$

> _C1:=1e-7;

$$_C1 := .1\ 10^{-6}$$

> c2(x);

$$.1\ 10^{-6}$$

> u2(x);

$$-.00169340357351905\ x + 2.50000000000000\ x\ _C2 + 1.00000000000000\ _C3$$

> S2(x);

$$.500000000000001\ 10^{12}\ _C2 - .390785440042860\ 10^{9}$$

> _C2:=solve(S2(0.1)=0.0,_C2);

$$_C2 := .000781570880085718$$

> S2(x);

$$0$$

> u2(x);

$$.000260523626695245\ x + 1.00000000000000\ _C3$$

> _C3:=solve(u2(0.0)=0,_C3);

$$_C3 := 0$$

> u2(x);

$$.000260523626695245\ x$$

> e2(x);

$$.000781570880085718$$

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#2a.ms

==========

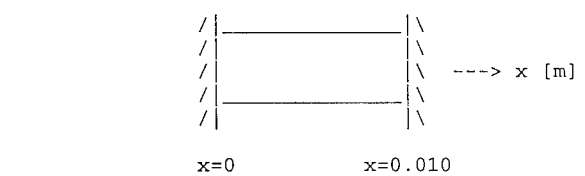
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, u(0.10)=0
Concentration variable boundary conditions: c(0)=0, c(0.10)=1e-6
Reference concentration level: c0=0.0
Trapping parameter: traps=19 (low trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=diff(J,x)=0;

$$deqn := Ds\,K1\,K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)^2 + Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial^2}{\partial x^2}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} - \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2},$$

$$\mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} + \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2}$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         boundary conditions will be used to select the proper one.
```

> c1:=unapply(simplify(op(2,csoln[1])),x);

$$c1 := x \rightarrow \frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c1(x);

$$\frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow -\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2(x);

$$-\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> J1:=unapply(simplify(Ds*(K1*K2*c1(x)-1)*diff(c1(x),x),x));

$$J1 := (\,) \rightarrow Ds\,_C1$$

> J1(x);

$$Ds\,_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := (\,) \rightarrow Ds\,_C1$$

> J2(x);

$$Ds\,_C1$$

Note #2: The above results show that both mass flux solutions are identical and equal to Ds*_C1 where _C1 is a constant of integration!

> ex1:=dsolve(diff(e(x),x)-K2*diff(c1(x),x)=0,e(x));

$$ex1 := \mathrm{e}(x) = \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1:=unapply(simplify(op(2,ex1)),x);

$$e1 := x \rightarrow \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1(x);

$$\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> ex2:=dsolve(diff(e(x),x)-K2*diff(c2(x),x)=0,e(x));

$$ex2 := \mathrm{e}(x) = \frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e2:=unapply(simplify(op(2,ex2)),x);

$$e2 := x \rightarrow \frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e2(x);

$$\frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

```
> ux1:=dsolve(A1*diff(u(x),x)+A2*c1(x)-A3-e1(x)=0,u(x));
```

$$ux1 := u(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> u1:=unapply(simplify(op(2,ux1)),x);
```

$$u1 := x \to \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2 + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,x + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

```
> u1(x);
```

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));
```

$$ux2 := u(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> u2:=unapply(simplify(op(2,ux2)),x);

$$u2 := x \rightarrow \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\right.$$
$$+ 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,x$$
$$+ 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1$$
$$- \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;K2$$
$$- 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,x$$
$$- 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1$$
$$\left. + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)\Big/(A1\,K1^2\,K2^2\,_C1)$$

> u2(x);

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,_C2\right.$$
$$+ 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\;K2 - 2\sqrt{\%1}\;K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\;K2^2\,K1\,_C1\,_C2$$
$$\left. + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)\Big/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> S1:=x->simplify(B1*e1(x)-B2*c1(x)+B3);

$$S1 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e1}(x) - B2\;\mathrm{c1}(x) + B3)$$

> S1(x);

$$\left(B1\,K2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B1\,K2\,_C3\,K1 - B2\right.$$
$$\left. - B2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B3\,K1\,K2\right)\Big/(K1\,K2)$$

> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);

$$S2 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e2}(x) - B2\;\mathrm{c2}(x) + B3)$$

> S2(x);

$$\left(-B1\,K2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B1\,K2\,_C3\,K1 - B2\right.$$
$$\left. + B2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B3\,K1\,K2\right)\Big/(K1\,K2)$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

> K:=(Em/(3*(1-2*nu)));

$$K := \frac{Em}{3 - 6\,\nu}$$

> lambda:=(Em*nu)/((1+nu)*(1-2*nu));

$$\lambda := \frac{Em\,\nu}{(1 + \nu)(1 - 2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2 + 2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\,\frac{\rho\, Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\, Em}{(3 - 6\,\nu)\, R\, T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\, Vs\, (1 + traps)}{MWs}$$

```
> K1*K2;
```

$$\frac{Vs^2\, Em\, \rho\, (1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\,\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\,\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)\, c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\,\frac{Em\, \rho\, Vs\, (1 + traps)}{(3 - 6\,\nu)\, MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\,\frac{Em\, \rho\, Vs\, (1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c1(x);

$$\left(1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T\,MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> c2(x);

$$-\left(-1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T\,MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> e1(x);

$$\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> e2(x);

$$\left(-\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> u1(x);

$$\frac{1}{3}\left(-2\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}-\frac{2}{3}\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$

$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+2\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}+\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$

$$+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$\left.+3\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\left((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\right)$$

$$\%1 := 1 + 2\frac{Vs^2\ Em\ \rho\ (1 + traps)\ _C1\ x}{(3 - 6\nu)\ R\ T\ MWs} + 2\frac{Vs^2\ Em\ \rho\ (1 + traps)\ _C1\ _C2}{(3 - 6\nu)\ R\ T\ MWs}$$

> u2(x);

$$\frac{1}{3}\left(-2\,\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em_C1}{MWs^2\,(3-6\,\nu)\,R\,T}+\frac{2}{3}\,\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\,\sqrt{\%1}}{MWs}\right.$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+2\,\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}-\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$

$$-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+3\,\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\,\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}$$

$$\left.\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\Big((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\Big)$$

$$\%1 := 1+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}$$

> S1(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

> S2(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

> S1(x)-S2(x);

$$0$$

Note #4: The stresses are same for each solution root, and do not depend on the position x! The stresses are therefore constant throughout the body. We define a new stress function, Sx.

> Sx:=S2(x);

$$Sx := -(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

Note #5: Now we will introduce numerical values for the material properties.
The values selected are typical for internal hydrogen as a
solute in AISI 4340 steel.

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=19;

$$traps := 19$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$312.628352034286$$

> K1*K2;

$$43205.0114421104$$

> 1/(K1*K2);

$$.0000231454631447068$$

> A1;

$$.4$$

> A2;

$$270.944571763048$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.156314176017143\ 10^{15}$$

> B3;

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, _C3, and _C4, using the boundary data.

> c1(x);

$$.0000231454631447068 + \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> c2(x);

$$.0000231454631447068 - \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> evalf(c1(x),5);

$$.000023146 + \frac{.000023146}{\sqrt{1. + 86408.\ _C1\ x + 86408.\ _C1\ _C2}}$$

> evalf(c2(x),5);

$$.000023146 - \frac{.000023146}{\sqrt{1. + 86408.\ _C1\ x + 86408.\ _C1\ _C2}}$$

> eqnset1:={0=c1(0),1e-6=c1(0.10)};

$$eqnset1 := \left\{ .1\ 10^{-5} = .0000231454631447068 + \frac{.0000231454631447068}{\sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}}, 0 = .0000231454631447068 + \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ _C2}} \right\}$$

> varset1:={_C1,_C2};

$$varset1 := \{ _C1, _C2 \}$$

> solnset1:=solve(eqnset1,varset1);

$$solnset1 :=$$

> eqnset2:={0=c2(0),1e-6=c2(0.10)};

$$eqnset2 := \left\{ 0 = .0000231454631447068 - \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ _C2}}, \right.$$

$$.1\ 10^{-5} = .0000231454631447068$$

$$- .0000231454631447068 \sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}$$

$$\}$$

```
> varset2:={_C1,_C2};
```

$$varset2 := \{_C1, _C2\}$$

```
> solnset2:=solve(eqnset2,varset2);
```

$$solnset2 := \{_C2 = 0, _C1 = -.978397494278943\ 10^{-5}\}$$

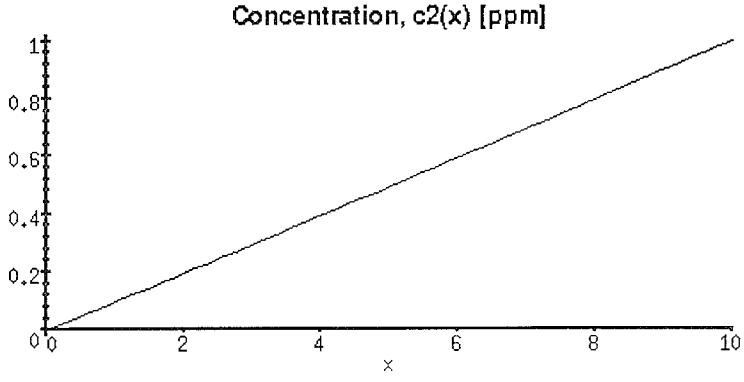
```
> assign(solnset2);
```

```
Note #7: The solution c1(x) is not capable of satisfying the boundary
         conditions, as evidenced by the lack of solution for the given
         boundary conditions. The concentration function c2(x) is the
         correct solution in this case!
```

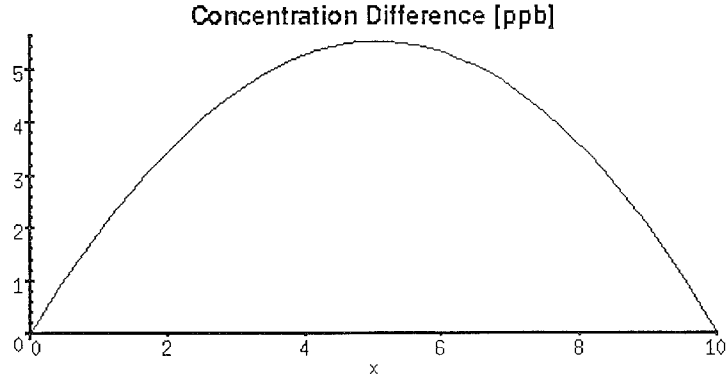
```
> c2(x);
```

$$.0000231454631447068 - .0000231454631447068 \sqrt{1 - .845433498705078\ x}$$

```
> p1:=plot(1e6*c2(x/100),x=0..10,title='Concentration, c2(x) [ppm]'):
> p1;
>
```




```
> p2:=plot(1e9*(c2(0)+((c2(0.10)-c2(0))/0.10)*x/100-c2(x/100)),x=0..10,title='Concentration Difference [ppb]'):
> p2;
>
```



```
> u2(x);
```

$$-.0156778439999998\,x + .00190196390663828\,\sqrt{1 - .845433498705078\,x} - .00160798400000005\,\sqrt{1 - .845433498705078\,x}\,x + 2.49999999999998\,_C3\,x + .999999999999996\,_C4$$

```
> eqnset3:={0=u2(0),0=u2(0.10)};
```

$$eqnset3 := \{\, 0 = .000098154031001431 6 + .249999999999998\,_C3 + .999999999999996\,_C4,\ 0 = .00190196390663828 + .999999999999996\,_C4 \,\}$$

```
> varset3:={_C3,_C4};
```

$$varset3 := \{\, _C3, _C4 \,\}$$

```
> solnset3:=solve(eqnset3,varset3);
```

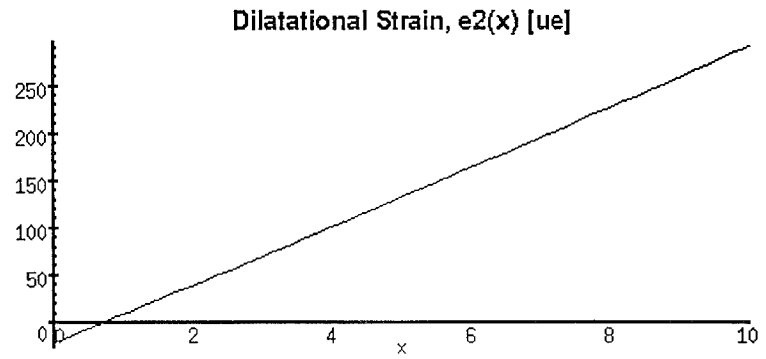
$$solnset3 := \{\, _C3 = .00721523950254741,\ _C4 = -.00190196390663828 \,\}$$

```
> assign(solnset3);
```

```
> e2(x);
```

$$-.00723592799999998\,\sqrt{1 - .845433498705078\,x} + .00721523950254741$$

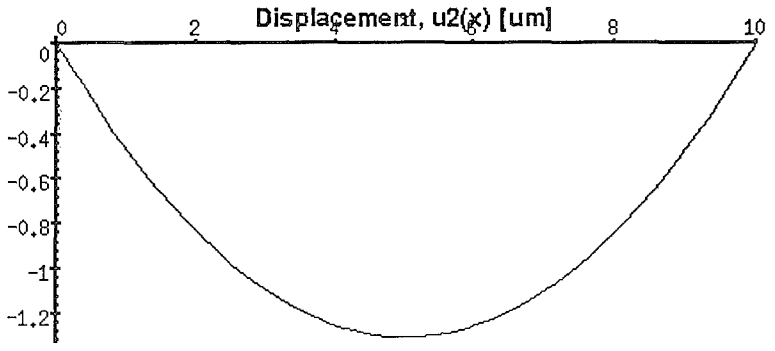
```
> p3:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p3;
>
```



```
> u2(x);
```

$$.00236025475636850\,x + .00190196390663828\,\sqrt{1 - .845433498705078\,x} - .00160798400000005\,\sqrt{1 - .845433498705078\,x}\,x - .00190196390663825$$

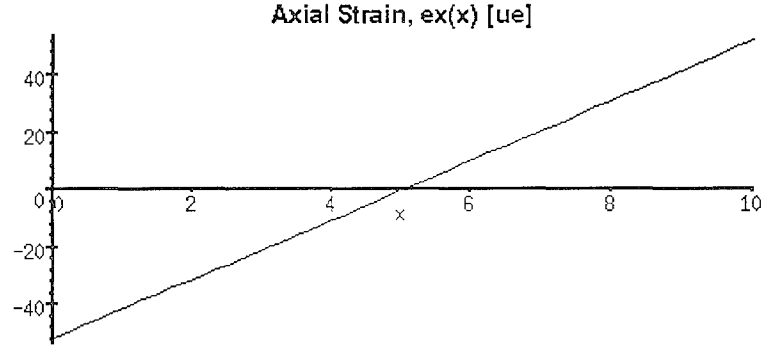
```
> p4:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p4;
>
```




```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := x \rightarrow .00236025475636850 - .000803991999999990 \frac{1}{\sqrt{1 - .845433498705078\, x}} + .000679721769490914 \frac{x}{\sqrt{1 - .845433498705078\, x}} - .00160798400000005 \sqrt{1 - .845433498705078\, x}$$

```
> p5:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p5;
>
```



```
> Sx;
```

$$-.103442487262901\ 10^{8}$$

```
> J2(x);
```

$$-.978397494278943\ 10^{-14}$$

```
> evalf(u2(x),5);
```

$$.0023588\,x + .0019015\sqrt{1. - .84542\,x} - .0016072\sqrt{1. - .84542\,x}\,x - .0019021$$

```
> evalf(c2(x),5);
```

$$.000023146 - .000023146\sqrt{1. - .84542\,x}$$

```
> evalf(e2(x),5);
```

$$-.0072359\sqrt{1. - .84542\,x} + .0072152$$

```
> evalf(ex(x),5);
```

$$.0023603 - .00080399\frac{1}{\sqrt{1. - .84543\,x}} + .00067972\frac{x}{\sqrt{1. - .84543\,x}} - .0016080\sqrt{1. - .84543\,x}$$

```
>
```

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#2b.ms

==========

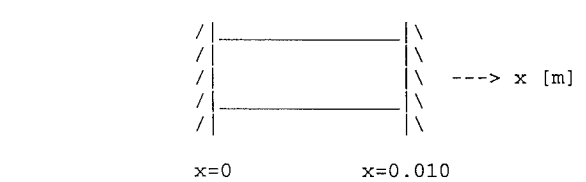
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, u(0.10)=0
Concentration variable boundary conditions: c(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=19 (low trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=diff(J,x)=0;

$$deqn := Ds\,K1\,K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)^2 + Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial^2}{\partial x^2}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} - \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2},$$

$$\mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} + \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2}$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         boundary conditions will be used to select the proper one.
```

> c1:=unapply(simplify(op(2,csoln[1])),x);

$$c1 := x \rightarrow \frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c1(x);

$$\frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow -\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2(x);

$$-\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> J1:=unapply(simplify(Ds*(K1*K2*c1(x)-1)*diff(c1(x),x),x));

$$J1 := (\,) \rightarrow Ds\,_C1$$

> J1(x);

$$Ds\,_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := (\,) \rightarrow Ds\,_C1$$

> J2(x);

$$Ds\,_C1$$

Note #2: The above results show that both mass flux solutions are identical and equal to Ds*_C1 where _C1 is a constant of integration!

> ex1:=dsolve(diff(e(x),x)-K2*diff(c1(x),x)=0,e(x));

$$ex1 := \mathrm{e}(x) = \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1:=unapply(simplify(op(2,ex1)),x);

$$e1 := x \rightarrow \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1(x);

$$\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> ex2:=dsolve(diff(e(x),x)-K2*diff(c2(x),x)=0,e(x));

$$ex2 := \mathrm{e}(x) = -\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-_C3\,K1}{K1}$$

> e2:=unapply(simplify(op(2,ex2)),x);

$$e2 := x \rightarrow \frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e2(x);

$$\frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

```
> ux1:=dsolve(A1*diff(u(x),x)+A2*c1(x)-A3-e1(x)=0,u(x));
```

$$ux1 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> u1:=unapply(simplify(op(2,ux1)),x);
```

$$u1 := x \to \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2 + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,x + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

```
> u1(x);
```

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

```
> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));
```

$$ux2 := \mathrm{u}(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> u2:=unapply(simplify(op(2,ux2)),x);

$$u2 := x \rightarrow \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\right.$$
$$+ 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,x$$
$$+ 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1$$
$$- \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;K2$$
$$- 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,x$$
$$- 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1$$
$$\left. + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)\Big/(A1\,K1^2\,K2^2\,_C1)$$

> u2(x);

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,_C2\right.$$
$$+ 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\;K2 - 2\sqrt{\%1}\;K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\;K2^2\,K1\,_C1\,_C2$$
$$\left. + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)\Big/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> S1:=x->simplify(B1*e1(x)-B2*c1(x)+B3);

$$S1 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e1}(x) - B2\;\mathrm{c1}(x) + B3)$$

> S1(x);

$$\left(B1\,K2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B1\,K2\,_C3\,K1 - B2\right.$$
$$\left. - B2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B3\,K1\,K2\right)\Big/(K1\,K2)$$

> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);

$$S2 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e2}(x) - B2\;\mathrm{c2}(x) + B3)$$

> S2(x);

$$\left(-B1\,K2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B1\,K2\,_C3\,K1 - B2\right.$$
$$\left. + B2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + B3\,K1\,K2\right)\Big/(K1\,K2)$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

> K:=(Em/(3*(1-2*nu)));

$$K := \frac{Em}{3 - 6\,\nu}$$

> lambda:=(Em*nu)/((1+nu)*(1-2*nu));

$$\lambda := \frac{Em\,\nu}{(1 + \nu)(1 - 2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2 + 2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\,\frac{\rho\, Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\, Em}{(3 - 6\,\nu)\, R\, T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\, Vs\,(1 + traps)}{MWs}$$

```
> K1*K2;
```

$$\frac{Vs^2\, Em\, \rho\,(1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\,\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\,\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)\, c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)}{(3 - 6\,\nu)\, MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c1(x);

$$\left(1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs/(Vs^2\,Em\,\rho\,(1+traps))$$

> c2(x);

$$-\left(-1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs/(Vs^2\,Em\,\rho\,(1+traps))$$

> e1(x);

$$\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T/(Vs\,Em)$$

> e2(x);

$$\left(-\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T/(Vs\,Em)$$

> u1(x);

$$\frac{1}{3}\left(-2\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}-\frac{2}{3}\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$
$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$-\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$+2\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}+\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$
$$+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}+2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$+3\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}$$
$$\left.\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2/\left((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\right)$$

$$\%1 := 1 + 2\,\frac{Vs^2\ Em\ \rho\ (1 + traps)\ _C1\ x}{(3 - 6\,\nu)\ R\ T\ MWs} + 2\,\frac{Vs^2\ Em\ \rho\ (1 + traps)\ _C1\ _C2}{(3 - 6\,\nu)\ R\ T\ MWs}$$

> u2(x);

$$\frac{1}{3}\left(-2\,\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em_C1}{MWs^2\,(3-6\,\nu)\,R\,T}+\frac{2}{3}\,\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\,\sqrt{\%1}}{MWs}\right.$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+2\,\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}-\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$

$$-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+3\,\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\,\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}$$

$$\left.\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\Big((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\Big)$$

$$\%1 := 1+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}$$

> S1(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

> S2(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

> S1(x)-S2(x);

$$0$$

```
Note #4: The stresses are same for each solution root, and do not depend on
         the position x! The stresses are therefore constant throughout the
         body. We define a new stress function, Sx.
```

> Sx:=S2(x);

$$Sx := -(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

Note #5: Now we will introduce numerical values for the material properties.
The values selected are typical for internal hydrogen as a
solute in AISI 4340 steel.

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=19;

$$traps := 19$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$312.628352034286$$

> K1*K2;

$$43205.0114421104$$

> 1/(K1*K2);

$$.0000231454631447068$$

> A1;

$$.4$$

> A2;

$$270.944571763048$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.156314176017143\ 10^{15}$$

> B3;

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, _C3, and _C4, using the boundary data.

> c1(x);

$$.0000231454631447068 + \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> c2(x);

$$.0000231454631447068 - \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ x + 86410.0228842208\ _C1\ _C2}}$$

> evalf(c1(x),5);

$$.000023146 + \frac{.000023146}{\sqrt{1. + 86408.\ _C1\ x + 86408.\ _C1\ _C2}}$$

> evalf(c2(x),5);

$$.000023146 - \frac{.000023146}{\sqrt{1. + 86408.\ _C1\ x + 86408.\ _C1\ _C2}}$$

> eqnset1:={0=c1(0),1e-7=c1(0.10)};

$$eqnset1 := \left\{ .1\ 10^{-6} = .0000231454631447068 + \frac{.0000231454631447068}{\sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}}, 0 = .0000231454631447068 + \frac{.0000231454631447068}{\sqrt{1 + 86410.0228842208\ _C1\ _C2}} \right\}$$

> varset1:={_C1,_C2};

$$varset1 := \{ _C1, _C2 \}$$

> solnset1:=solve(eqnset1,varset1);

$$solnset1 :=$$

> eqnset2:={0=c2(0),1e-7=c2(0.10)};

$$eqnset2 := \left\{ .1\ 10^{-6} = .0000231454631447068 - \frac{.0000231454631447068}{\sqrt{1 + 8641.00228842208\ _C1 + 86410.0228842208\ _C1\ _C2}} \right.$$

$$, 0 =$$

$$.0000231454631447068 - .0000231454631447068\sqrt{1 + 86410.0228842208\ _C1\ _C2}\ \}$$

```
> varset2:={_C1,_C2};
```

$$varset2 := \{_C1, _C2\}$$

```
> solnset2:=solve(eqnset2,varset2);
```

$$solnset2 := \{_C2 = 0, _C1 = -.997839749427893\ 10^{-6}\}$$

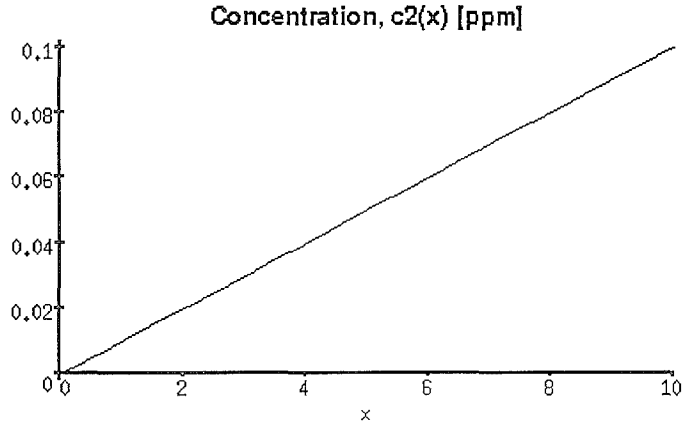
```
> assign(solnset2);
```

```
  Note #7: The solution c1(x) is not capable of satisfying the boundary
           conditions, as evidenced by the lack of solution for the given
           boundary conditions. The concentration function c2(x) is the
           correct solution in this case!
```

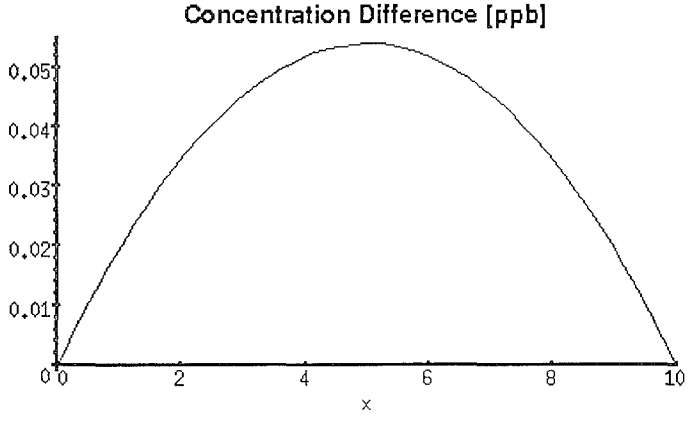
```
> c2(x);
```

$$.0000231454631447068 - .0000231454631447068\sqrt{1 - .0862233555828494\ x}$$

```
> p1:=plot(1e6*c2(x/100),x=0..10,title='Concentration, c2(x) [ppm]'):
> p1;
>
```




```
> p2:=plot(1e9*(c2(0)+((c2(0.10)-c2(0))/0.10)*x/100-c2(x/100)),x=0..10,title='Concentration Difference [ppb]'):
> p2;
>
```



```
> u2(x);
```

$$-.0156778440000000\,x + .0186490538338527\sqrt{1 - .0862233555828494\,x} - .00160798400000002\sqrt{1 - .0862233555828494\,x}\,x + 2.49999999999999\,_C3\,x + .999999999999992\,_C4$$

```
> eqnset3:={0=u2(0),0=u2(0.10)};
```

$$eqnset3 := \{\, 0 = .0186490538338527 + .999999999999992\,_C4,\ 0 = .0168405925050965 + .249999999999999\,_C3 + .999999999999992\,_C4 \,\}$$

```
> varset3:={_C3,_C4};
```

$$varset3 := \{\, _C3, _C4 \,\}$$

```
> solnset3:=solve(eqnset3,varset3);
```

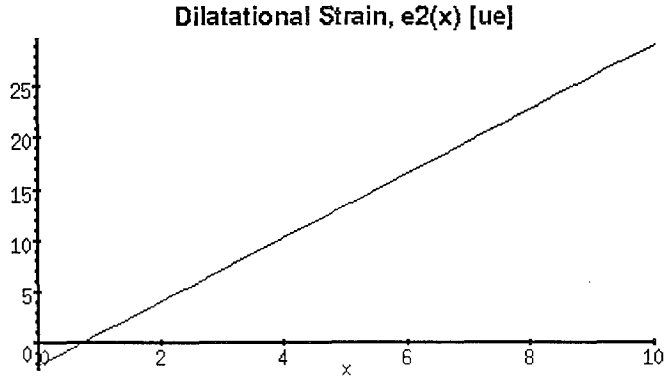
$$solnset3 := \{\, _C3 = .00723384531502524,\ _C4 = -.0186490538338529 \,\}$$

```
> assign(solnset3);
```

```
> e2(x);
```

$$-.00723592799999998\sqrt{1 - .0862233555828494\,x} + .00723384531502525$$

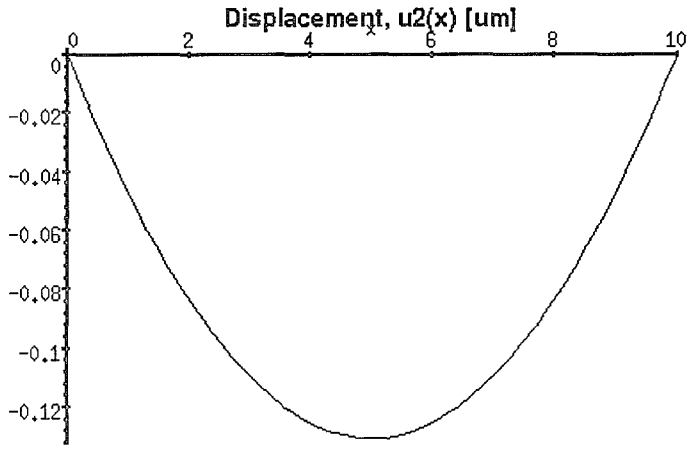
```
> p3:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p3;
>
```



```
> u2(x);
```

$$.00240676928756317\,x + .0186490538338527\sqrt{1 - .0862233555828494\,x} - .00160798400000002\sqrt{1 - .0862233555828494\,x}\,x - .0186490538338527$$

```
> p4:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p4;
>
```



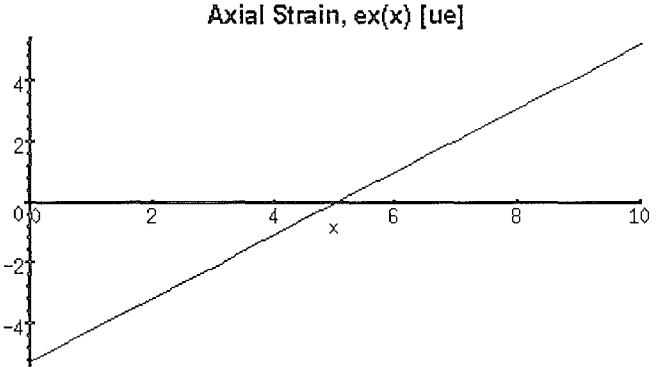

```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := x \rightarrow .00240676928756317 - .000803991999999991 \frac{1}{\sqrt{1 - .0862233555828494\,x}}$$

$$+ .0000693228881017671 \frac{x}{\sqrt{1 - .0862233555828494\,x}}$$

$$- .00160798400000002 \sqrt{1 - .0862233555828494\,x}$$

```
> p5:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p5;
>
```



> Sx;

$$-.104134248738053\ 10^{7}$$

> J2(x);

$$-.997839749427893\ 10^{-15}$$

> evalf(u2(x),5);

$$.0024067\,x + .018644\sqrt{1. - .086222\,x} - .0016072\sqrt{1. - .086222\,x}\,x - .018650$$

> evalf(c2(x),5);

$$.000023146 - .000023146\sqrt{1. - .086222\,x}$$

> evalf(e2(x),5);

$$-.0072359\sqrt{1. - .086222\,x} + .0072338$$

> evalf(ex(x),5);

$$.0024068 - .00080399\frac{1}{\sqrt{1. - .086223\,x}} + .000069323\frac{x}{\sqrt{1. - .086223\,x}} - .0016080\sqrt{1. - .086223\,x}$$

---

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#2c.ms

==========

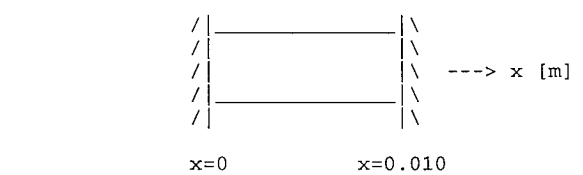
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, u(0.10)=0
Concentration variable boundary conditions: c(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=499 (high trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=diff(J,x)=0;

$$deqn := Ds\,K1\,K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)^2 + Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial^2}{\partial x^2}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} - \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2},$$

$$\mathrm{c}(x) = -\frac{_C1\left(-\frac{1}{_C1} + \frac{\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{_C1}\right)}{K1\,K2}$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         boundary conditions will be used to select the proper one.
```

> c1:=unapply(simplify(op(2,csoln[1])),x);

$$c1 := x \rightarrow \frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c1(x);

$$\frac{1 + \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow -\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> c2(x);

$$-\frac{-1+\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}}{K1\,K2}$$

> J1:=unapply(simplify(Ds*(K1*K2*c1(x)-1)*diff(c1(x),x),x));

$$J1 := (\,) \rightarrow Ds\,_C1$$

> J1(x);

$$Ds\,_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := (\,) \rightarrow Ds\,_C1$$

> J2(x);

$$Ds\,_C1$$

Note #2: The above results show that both mass flux solutions are identical
and equal to Ds*_C1 where _C1 is a constant of integration!

> ex1:=dsolve(diff(e(x),x)-K2*diff(c1(x),x)=0,e(x));

$$ex1 := \mathrm{e}(x) = \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1:=unapply(simplify(op(2,ex1)),x);

$$e1 := x \rightarrow \frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e1(x);

$$\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> ex2:=dsolve(diff(e(x),x)-K2*diff(c2(x),x)=0,e(x));

$$ex2 := \mathrm{e}(x) = \frac{-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+_C3\,K1}{K1}$$

> e2:=unapply(simplify(op(2,ex2)),x);

$$e2 := x \rightarrow -\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-_C3\,K1}{K1}$$

> e2(x);

$$-\frac{\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-_C3\,K1}{K1}$$

> ux1:=dsolve(A1*diff(u(x),x)+A2*c1(x)-A3-e1(x)=0,u(x));

$$ux1 := u(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 - A2\sqrt{\%1} - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x - 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 + \sqrt{\%1}\,K2 + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x + 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> u1:=unapply(simplify(op(2,ux1)),x);

$$u1 := x \to -\frac{1}{3}\left(3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2} + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,A2\,K1\,K2\,_C1\,_C2 - 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2 - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,x - 2\sqrt{1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2}\,K2^2\,K1\,_C1\,_C2 - 3\,_C3\,x\,K1^2\,K2^2\,_C1 - 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

> u1(x);

$$-\frac{1}{3}\left(3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 - 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 - 3\,_C3\,x\,K1^2\,K2^2\,_C1 - 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));

$$ux2 := u(x) = \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1} + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,x + 2\sqrt{\%1}\,A2\,K1\,K2\,_C1\,_C2 + 3\,A3\,x\,K1^2\,K2^2\,_C1 - \sqrt{\%1}\,K2 - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,x - 2\sqrt{\%1}\,K2^2\,K1\,_C1\,_C2 + 3\,_C3\,x\,K1^2\,K2^2\,_C1 + 3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1 + 2\,K1\,K2\,_C1\,x + 2\,K1\,K2\,_C1\,_C2$$

> u2:=unapply(simplify(op(2,ux2)),x);

$$u2 := x \rightarrow \frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\right.$$
$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,x$$
$$+2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;A2\,K1\,K2\,_C1\,_C2+3\,A3\,x\,K1^2\,K2^2\,_C1$$
$$-\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,x$$
$$-2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}\;K2^2\,K1\,_C1\,_C2+3\,_C3\,x\,K1^2\,K2^2\,_C1$$
$$\left.+3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)\Big/(A1\,K1^2\,K2^2\,_C1)$$

> u2(x);

$$\frac{1}{3}\left(-3\,A2\,x\,K1\,K2\,_C1 + A2\sqrt{\%1}+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,x+2\sqrt{\%1}\;A2\,K1\,K2\,_C1\,_C2\right.$$
$$+3\,A3\,x\,K1^2\,K2^2\,_C1-\sqrt{\%1}\;K2-2\sqrt{\%1}\;K2^2\,K1\,_C1\,x-2\sqrt{\%1}\;K2^2\,K1\,_C1\,_C2$$
$$\left.+3\,_C3\,x\,K1^2\,K2^2\,_C1+3\,_C4\,A1\,K1^2\,K2^2\,_C1\right)\Big/(A1\,K1^2\,K2^2\,_C1)$$

$$\%1 := 1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2$$

> S1:=x->simplify(B1*e1(x)-B2*c1(x)+B3);

$$S1 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e1}(x) - B2\;\mathrm{c1}(x) + B3)$$

> S1(x);

$$\left(B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B1\,K2\,_C3\,K1-B2\right.$$
$$\left.-B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}+B3\,K1\,K2\right)\Big/(K1\,K2)$$

> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);

$$S2 := x \rightarrow \mathrm{simplify}(B1\;\mathrm{e2}(x) - B2\;\mathrm{c2}(x) + B3)$$

> S2(x);

$$-\left(B1\,K2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-B1\,K2\,_C3\,K1+B2\right.$$
$$\left.-B2\sqrt{1+2\,K1\,K2\,_C1\,x+2\,K1\,K2\,_C1\,_C2}-B3\,K1\,K2\right)\Big/(K1\,K2)$$

Note #3: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

> K:=(Em/(3*(1-2*nu)));

$$K := \frac{Em}{3 - 6\,\nu}$$

> lambda:=(Em*nu)/((1+nu)*(1-2*nu));

$$\lambda := \frac{Em\,\nu}{(1+\nu)\,(1-2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2 + 2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\,\frac{\rho\, Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\, Em}{(3 - 6\,\nu)\, R\, T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\, Vs\,(1 + traps)}{MWs}$$

```
> K1*K2;
```

$$\frac{Vs^2\, Em\, \rho\,(1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\,\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\,\frac{(1 + \nu)\,\rho\, Vs\,(1 + traps)\, c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)}{(3 - 6\,\nu)\, MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\,\frac{Em\,\rho\, Vs\,(1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c1(x);

$$\left(1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> c2(x);

$$-\left(-1+\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}\right)(3-6\,\nu)\,R\,T$$
$$MWs\Big/(Vs^2\,Em\,\rho\,(1+traps))$$

> e1(x);

$$\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}+\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> e2(x);

$$-\left(\sqrt{1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}}-\frac{_C3\,Vs\,Em}{(3-6\,\nu)\,R\,T}\right)$$
$$(3-6\,\nu)\,R\,T\Big/(Vs\,Em)$$

> u1(x);

$$-\frac{1}{3}\left(2\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}+\frac{2}{3}\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\sqrt{\%1}}{MWs}\right.$$
$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$+\frac{4}{3}\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$-2\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}-\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$
$$-2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}-2\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$
$$\left.-3\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}-3\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}\right)$$
$$(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\left((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\right)$$

$$\%1 := 1+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}$$

> u2(x);

$$\frac{1}{3}\left(-2\,\frac{(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,x\,Em\,_C1}{MWs^2\,(3-6\,\nu)\,R\,T}+\frac{2}{3}\,\frac{(1+\nu)\,\rho\,Vs\,(1+traps)\,\sqrt{\%1}}{MWs}\right.$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+\frac{4}{3}\,\frac{\sqrt{\%1}\,(1+\nu)\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+2\,\frac{(1+\nu)\,\rho^3\,Vs^5\,(1+traps)^3\,c0\,x\,Em^2\,_C1}{MWs^3\,(3-6\,\nu)^2\,R^2\,T^2}-\frac{\sqrt{\%1}\,\rho\,Vs\,(1+traps)}{MWs}$$

$$-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,x}{MWs^2\,(3-6\,\nu)\,R\,T}-2\,\frac{\sqrt{\%1}\,\rho^2\,Vs^3\,(1+traps)^2\,Em\,_C1\,_C2}{MWs^2\,(3-6\,\nu)\,R\,T}$$

$$+3\,\frac{_C3\,x\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}+3\,\frac{_C4\,(1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1}{(3-6\,\nu)^2\,R^2\,T^2\,MWs^2}$$

$$\left.\right)(3-6\,\nu)^2\,R^2\,T^2\,MWs^2\Big/\Big((1-2\,\nu)\,Vs^4\,Em^2\,\rho^2\,(1+traps)^2\,_C1\Big)$$

$$\%1 := 1+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,x}{(3-6\,\nu)\,R\,T\,MWs}+2\,\frac{Vs^2\,Em\,\rho\,(1+traps)\,_C1\,_C2}{(3-6\,\nu)\,R\,T\,MWs}$$

> S1(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

> S2(x);

$$-(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

> S1(x)-S2(x);

$$0$$

Note #4: The stresses are same for each solution root, and do not depend on the position x! The stresses are therefore constant throughout the body. We define a new stress function, Sx.

> Sx:=S2(x);

$$Sx := -(MWs\,_C3\,Vs\,Em-3\,R\,T\,MWs+6\,R\,T\,MWs\,\nu+Em\,\rho\,Vs^2\,c0+Em\,\rho\,Vs^2\,c0\,traps)\Big/(\,(-1+2\,\nu)\,Vs\,MWs)$$

Note #5: Now we will introduce numerical values for the material properties. The values selected are typical for internal hydrogen as a solute in AISI 4340 steel.

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=499;

$$traps := 499$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$7815.70880085715$$

> K1*K2;

$$.108012528605276\ 10^{7}$$

> 1/(K1*K2);

$$.925818525788271\ 10^{-6}$$

> A1;

$$.4$$

> A2;

$$6773.61429407620$$

> A3;

$$0$$

> B1;

$$.500000000000001\ 10^{12}$$

> B2;

$$.390785440042860\ 10^{16}$$

> B3;

$$0$$

Note #6: Now let's solve for the integration constants: _C1, _C2, _C3, and _C4, using the boundary data.

> c1(x);

$$.925818525788271\ 10^{-6} + .925818525788271\ 10^{-6} \sqrt{1 + .216025057210552\ 10^{7}\ _C1\ x + .216025057210552\ 10^{7}\ _C1\ _C2}$$

> c2(x);

$$.925818525788271\ 10^{-6} - .925818525788271\ 10^{-6} \sqrt{1 + .216025057210552\ 10^{7}\ _C1\ x + .216025057210552\ 10^{7}\ _C1\ _C2}$$

> evalf(c1(x),5);

$$.92584\ 10^{-6} + .92584\ 10^{-6} \sqrt{1. + .21602\ 10^{7}\ _C1\ x + .21602\ 10^{7}\ _C1\ _C2}$$

> evalf(c2(x),5);

$$.92584\ 10^{-6} - .92584\ 10^{-6} \sqrt{1. + .21602\ 10^{7}\ _C1\ x + .21602\ 10^{7}\ _C1\ _C2}$$

> eqnset1:={0=c1(0),1e-7=c1(0.10)};

$$eqnset1 := \left\{ 0 = .925818525788271\ 10^{-6} + .925818525788271\ 10^{-6} \sqrt{1 + .216025057210552\ 10^{7}\ _C1\ _C2}, .1\ 10^{-6} = .925818525788271\ 10^{-6} + .925818525788271\ 10^{-6} \sqrt{1 + 216025.057210552\ _C1 + .216025057210552\ 10^{7}\ _C1\ _C2} \right\}$$

> varset1:={_C1,_C2};

$$varset1 := \{ _C2, _C1 \}$$

> solnset1:=solve(eqnset1,varset1);

$$solnset1 :=$$

> eqnset2:={0=c2(0),1e-7=c2(0.10)};

$$eqnset2 := \left\{ .1\ 10^{-6} = .925818525788271\ 10^{-6} - .925818525788271\ 10^{-6} \sqrt{1 + 216025.057210552\ _C1 + .216025057210552\ 10^{7}\ _C1\ _C2}, 0 = \right.$$

$$.925818525788271\ 10^{-6}$$

$$-.925818525788271\ 10^{-6}\sqrt{1 + .216025057210552\ 10^{7}\ _C1\ _C2}\ \}$$

```
> varset2:={_C1,_C2};
```

$$varset2 := \{_C2, _C1\}$$

```
> solnset2:=solve(eqnset2,varset2);
```

$$solnset2 := \{_C2 = 0, _C1 = -.945993735697361\ 10^{-6}\}$$

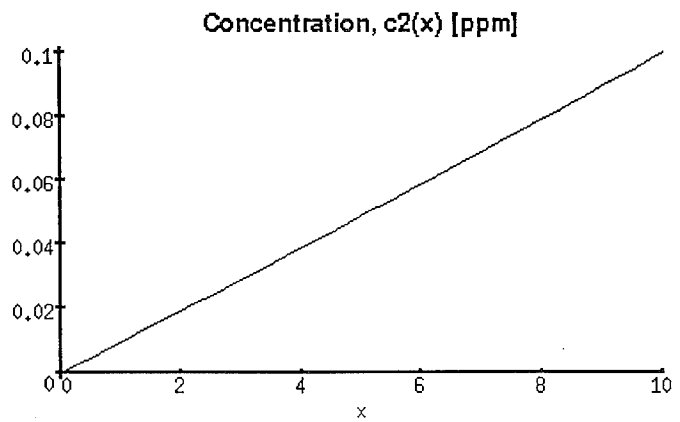
```
> assign(solnset2);
```

```
  Note #7: The solution c1(x) is not capable of satisfying the boundary
           conditions, as evidenced by the lack of solution for the given
           boundary conditions. The concentration function c2(x) is the
           correct solution in this case!
```

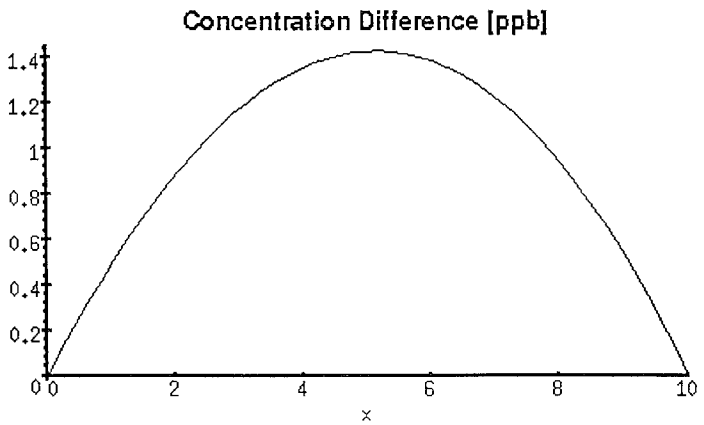
```
> c2(x);
```

$$.925818525788271\ 10^{-6} - .925818525788271\ 10^{-6}\sqrt{1 - 2.04358350874846\ x}$$

```
> p1:=plot(1e6*c2(x/100),x=0..10,title='Concentration, c2(x) [ppm]'):
> p1;
>
```




```
> p2:=plot(1e9*(c2(0)+((c2(0.10)-c2(0))/0.10)*x/100-c2(x/100)),x=0..10,title='Concentration Difference [ppb]'):
> p2;
>
```



```
> u2(x);
```

$$-.0156778440000000\,x + .000786845261334466\sqrt{1 - 2.04358350874846\,x} - .00160798399999998\sqrt{1 - 2.04358350874846\,x}\,x + 2.49999999999998\,_C3\,x + .999999999999996\,_C4$$

```
> eqnset3:={0=u2(0),0=u2(0.10)};
```

$$eqnset3 := \{\, 0 = .000786845261334466 + .999999999999996\,_C4,\; 0 = -.00100935844318366 + .249999999999998\,_C3 + .999999999999996\,_C4 \,\}$$

```
> varset3:={_C3,_C4};
```

$$varset3 := \{\, _C3, _C4 \,\}$$

```
> solnset3:=solve(eqnset3,varset3);
```

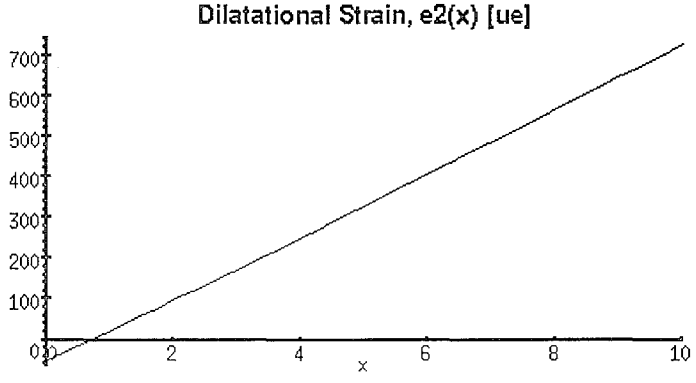
$$solnset3 := \{\, _C4 = -.000786845261334466,\; _C3 = .00718481481807253 \,\}$$

```
> assign(solnset3);
```

```
> e2(x);
```

$$-.00723592799999998\sqrt{1 - 2.04358350874846\,x} + .00718481481807253$$

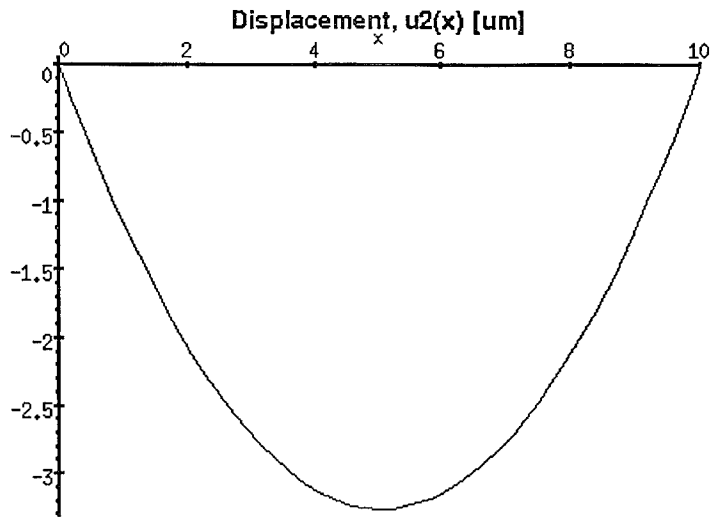
```
> p3:=plot(1e6*e2(x/100),x=0..10,title='Dilatational Strain, e2(x) [ue]'):
> p3;
>
```



```
> u2(x);
```

$$.00228419304518136\,x + .000786845261334466\sqrt{1 - 2.04358350874846\,x} - .00160798399999998\sqrt{1 - 2.04358350874846\,x}\,x - .000786845261334466$$

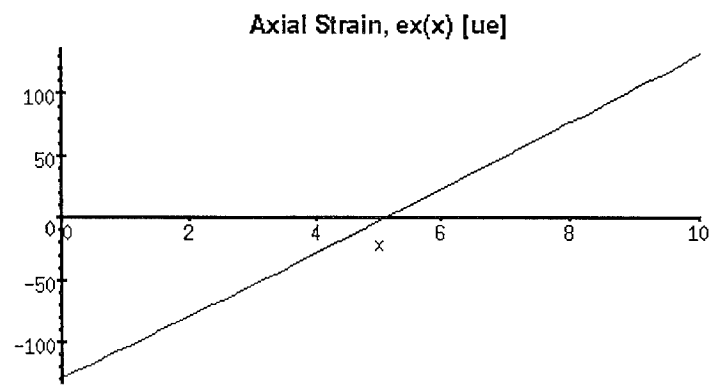
```
> p4:=plot(1e6*u2(x/100),x=0..10,title='Displacement, u2(x) [um]'):
> p4;
>
```



```
> ex:=unapply(diff(u2(x),x),x);
```

$$ex := x \rightarrow .00228419304518136 - .000803991999999993 \frac{1}{\sqrt{1 - 2.04358350874846\,x}} + .00164302479236567 \frac{x}{\sqrt{1 - 2.04358350874846\,x}} - .00160798399999998 \sqrt{1 - 2.04358350874846\,x}$$

```
> p5:=plot(1e6*ex(x/100),x=0..10,title='Axial Strain, ex(x) [ue]'):
> p5;
>
```



> Sx;

$$-.255565909637320\ 10^{8}$$

> J2(x);

$$-.945993735697361\ 10^{-15}$$

> evalf(u2(x),5);

$$.0022826\,x + .00078643\sqrt{1. - 2.0436\,x} - .0016069\sqrt{1. - 2.0436\,x}\,x - .00078689$$

> evalf(c2(x),5);

$$.92584\ 10^{-6} - .92584\ 10^{-6}\sqrt{1. - 2.0436\,x}$$

> evalf(e2(x),5);

$$-.0072359\sqrt{1. - 2.0436\,x} + .0071848$$

> evalf(ex(x),5);

$$.0022842 - .00080399\frac{1}{\sqrt{1. - 2.0436\,x}} + .0016430\frac{x}{\sqrt{1. - 2.0436\,x}} - .0016080\sqrt{1. - 2.0436\,x}$$

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#2d.ms

==========

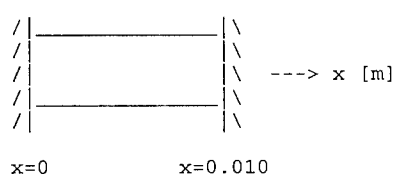
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, u(0.10)=0
Concentration variable boundary conditions: J(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=19 (low trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=J=0;

$$deqn := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = \frac{1}{K1\,K2},\ \mathrm{c}(x) = _C1$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         first solution is obviously incorrect in that the concentration
         throughout the rod is defined in terms of the constants K1 and K2.
         The second solution is adopted as correct.
```

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow _C1$$

> c2(x);

$$_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := 0$$

> J2(x);

$$0$$

```
Note #2: The above result shows that the mass flux is identically zero, as
         it should be.
```

Note #3: Since the concentration is constant, we have from the third governing equation that e(x) equals a constant.

```
> e2:=x->_C2;
```

$$e2 := x \rightarrow _C2$$

```
> e2(x);
```

$$_C2$$

```
> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));
```

$$ux2 := \mathrm{u}(x) = \frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

```
> u2:=unapply(simplify(op(2,ux2)),x);
```

$$u2 := x \rightarrow -\frac{x\,A2\,_C1 - x\,A3 - x\,_C2 - _C3\,A1}{A1}$$

```
> u2(x);
```

$$-\frac{x\,A2\,_C1 - x\,A3 - x\,_C2 - _C3\,A1}{A1}$$

```
> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);
```

$$S2 := x \rightarrow \mathrm{simplify}(B1\ \mathrm{e2}(x) - B2\ \mathrm{c2}(x) + B3)$$

```
> S2(x);
```

$$B1\,_C2 - B2\,_C1 + B3$$

Note #4: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

```
> K:=(Em/(3*(1-2*nu)));
```

$$K := \frac{Em}{3 - 6\,\nu}$$

```
> lambda:=(Em*nu)/((1+nu)*(1-2*nu));
```

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2 + 2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\,\frac{\rho\,Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\,Em}{(3 - 6\,\nu)\,R\,T}$$

> K2:=3*alpha*(1+traps);

$$K2 := \frac{\rho\, Vs\, (1 + traps)}{MWs}$$

> K1*K2;

$$\frac{Vs^2\, Em\, \rho\, (1 + traps)}{(3 - 6\,\nu)\, R\, T\, MWs}$$

> A1:=(1-2*nu);

$$A1 := 1 - 2\,\nu$$

> A2:=2*(1+nu)*alpha*(1+traps);

$$A2 := \frac{2}{3}\,\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)}{MWs}$$

> A3:=A2*c0;

$$A3 := \frac{2}{3}\,\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)\, c0}{MWs}$$

> B1:=3*K;

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

> B2:=9*K*alpha*(1+traps);

$$B2 := 3\,\frac{Em\, \rho\, Vs\, (1 + traps)}{(3 - 6\,\nu)\, MWs}$$

> B3:=B2*c0;

$$B3 := 3\,\frac{Em\, \rho\, Vs\, (1 + traps)\, c0}{(3 - 6\,\nu)\, MWs}$$

> c2(x);

$$_C1$$

> e2(x);

$$_C2$$

> collect(u2(x),x);

$$-\frac{\left(\frac{2}{3}\,\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)\, _C1}{MWs} - \frac{2}{3}\,\frac{(1 + \nu)\, \rho\, Vs\, (1 + traps)\, c0}{MWs} - _C2\right) x}{1 - 2\,\nu} + _C3$$

> S2(x);

$$\frac{Em\, (-_C2\, MWs + \rho\, Vs\, _C1 + \rho\, Vs\, _C1\, traps - \rho\, Vs\, c0 - \rho\, Vs\, c0\, traps)}{(-1 + 2\,\nu)\, MWs}$$

```
Note #5: Now we will introduce numerical values for the material properties.
         The values selected are typical for internal hydrogen as a
         solute in AISI 4340 steel.
```

```
> Ds:=1e-9;
```

$$Ds := .1\ 10^{-8}$$

```
> Vs:=2.02e-6;
```

$$Vs := .202\ 10^{-5}$$

```
> traps:=19;
```

$$traps := 19$$

```
> c0:=0.0;
```

$$c0 := 0$$

```
> MWs:=0.00100797;
```

$$MWs := .00100797$$

```
> Em:=200e9;
```

$$Em := .200\ 10^{12}$$

```
> nu:=0.3;
```

$$\nu := .3$$

```
> rho:=7800;
```

$$\rho := 7800$$

```
> T:=293;
```

$$T := 293$$

```
> R:=8.31432;
```

$$R := 8.31432$$

```
> K;
```

$$.166666666666667\ 10^{12}$$

```
> lambda;
```

$$.115384615384616\ 10^{12}$$

```
> mu;
```

$$.769230769230769\ 10^{11}$$

```
> alpha;
```

$$5.21047253390476$$

```
> Rh:=R/MWs;
```

$$Rh := 8248.57882675080$$

```
> K1;
```

$$138.199274509089$$

```
> K2;
```

$$312.628352034286$$

```
> K1*K2;
```

$$43205.0114421104$$

```
> 1/(K1*K2);
```

$$.0000231454631447068$$

```
> A1;
```

$$.4$$

```
> A2;
```

$$270.944571763048$$

```
> A3;
```

$$0$$

```
> B1;
```

$$.500000000000001\ 10^{12}$$

```
> B2;
```

$$.156314176017143\ 10^{15}$$

```
> B3;
```

$$0$$

```
  Note #6: Now let's solve for the integration constants: _C1, _C2, _C3, and _C4,
           using the boundary data.
```

```
> c2(x);
```

$$_C1$$

```
> _C1:=1e-7;
```

$$_C1 := .1\ 10^{-6}$$

```
> c2(x);
```

$$.1\ 10^{-6}$$

```
> u2(x);
```

$$-.0000677361429407620\ x + 2.50000000000000\ x\ _C2 + 1.00000000000000\ _C3$$

```
> eqnset1:={0.0=u2(0.0), 0.0=u2(0.10)};
```

$$eqnset1 := \{\ 0 = 1.00000000000000\ _C3,$$

$$0 = -.677361429407620\ 10^{-5} + .250000000000000\ _C2 + 1.00000000000000\ _C3\ \}$$

```
> varset1:={_C2,_C3};
```

$$varset1 := \{\ _C2, _C3\ \}$$

```
> solnset1:=solve(eqnset1,varset1);
```

$$solnset1 := \{\ _C3 = 0, _C2 = .0000270944571763048\ \}$$

```
> assign(solnset1);
```

```
> c2(x);
```

$$.1\ 10^{-6}$$

```
> e2(x);
```

$$.0000270944571763048$$

```
> u2(x);
```

$$0$$

```
> S2(x);
```

$$-.208418901356190\ 10^{7}$$

---

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#2e.ms

==========

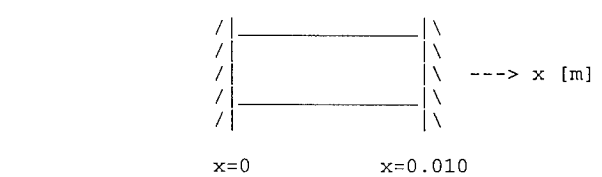
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: June-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem solved is shown below:



Deformation variable boundary conditions: u(0)=0, u(0.10)=0
Concentration variable boundary conditions: J(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: traps=499 (high trapping)

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx=0 (steady-state deformation equation with zero body forces)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

```
A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

> Digits:=trunc(evalhf(Digits));

$$Digits := 15$$

> J:=Ds*(K1*K2*c(x)-1)*diff(c(x),x);

$$J := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)$$

> deqn:=J=0;

$$deqn := Ds\,(K1\,K2\,\mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) = 0$$

> csoln:=dsolve(deqn,c(x),explicit);

$$csoln := \mathrm{c}(x) = \frac{1}{K1\,K2},\ \mathrm{c}(x) = _C1$$

```
Note #1: There are apparently two "roots" to the solution for c(x). The
         first solution is obviously incorrect in that the concentration
         throughout the rod is defined in terms of the constants K1 and K2.
         The second solution is adopted as correct.
```

> c2:=unapply(simplify(op(2,csoln[2])),x);

$$c2 := x \rightarrow _C1$$

> c2(x);

$$_C1$$

> J2:=unapply(simplify(Ds*(K1*K2*c2(x)-1)*diff(c2(x),x)));

$$J2 := 0$$

> J2(x);

$$0$$

```
Note #2: The above result shows that the mass flux is identically zero, as
         it should be.
```

Note #3: Since the concentration is constant, we have from the third governing equation that e(x) equals a constant.

```
> e2:=x->_C2;
```

$$e2 := x \rightarrow _C2$$

```
> e2(x);
```

$$_C2$$

```
> ux2:=dsolve(A1*diff(u(x),x)+A2*c2(x)-A3-e2(x)=0,u(x));
```

$$ux2 := \mathrm{u}(x) = \frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

```
> u2:=unapply(simplify(op(2,ux2)),x);
```

$$u2 := x \rightarrow \frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

```
> u2(x);
```

$$\frac{-x\,A2\,_C1 + x\,A3 + x\,_C2 + _C3\,A1}{A1}$$

```
> S2:=x->simplify(B1*e2(x)-B2*c2(x)+B3);
```

$$S2 := x \rightarrow \mathrm{simplify}(B1\ \mathrm{e2}(x) - B2\ \mathrm{c2}(x) + B3)$$

```
> S2(x);
```

$$B1\ _C2 - B2\ _C1 + B3$$

Note #4: At this point, we will introduce expressions for the constants and then simplify the results before quantifying the constants and determining the constants of integration.

```
> K:=(Em/(3*(1-2*nu)));
```

$$K := \frac{Em}{3 - 6\,\nu}$$

```
> lambda:=(Em*nu)/((1+nu)*(1-2*nu));
```

$$\lambda := \frac{Em\,\nu}{(1+\nu)\,(1-2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2 + 2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\,\frac{\rho\,Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\,Em}{(3 - 6\,\nu)\,R\,T}$$

> K2:=3*alpha*(1+traps);

$$K2 := \frac{\rho\ Vs\ (1 + traps)}{MWs}$$

> K1*K2;

$$\frac{Vs^2\ Em\ \rho\ (1 + traps)}{(3 - 6\ \nu)\ R\ T\ MWs}$$

> A1:=(1-2*nu);

$$A1 := 1 - 2\ \nu$$

> A2:=2*(1+nu)*alpha*(1+traps);

$$A2 := \frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)}{MWs}$$

> A3:=A2*c0;

$$A3 := \frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ c0}{MWs}$$

> B1:=3*K;

$$B1 := 3\ \frac{Em}{3 - 6\ \nu}$$

> B2:=9*K*alpha*(1+traps);

$$B2 := 3\ \frac{Em\ \rho\ Vs\ (1 + traps)}{(3 - 6\ \nu)\ MWs}$$

> B3:=B2*c0;

$$B3 := 3\ \frac{Em\ \rho\ Vs\ (1 + traps)\ c0}{(3 - 6\ \nu)\ MWs}$$

> c2(x);

$$_C1$$

> e2(x);

$$_C2$$

> collect(u2(x),x);

$$\frac{\left(-\frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ _C1}{MWs} + \frac{2}{3}\ \frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ c0}{MWs} + _C2\right) x}{1 - 2\ \nu} + _C3$$

> S2(x);

$$-\frac{Em\ (_C2\ MWs - \rho\ Vs\ _C1 - \rho\ Vs\ _C1\ traps + \rho\ Vs\ c0 + \rho\ Vs\ c0\ traps)}{(-1 + 2\ \nu)\ MWs}$$

Note #5: Now we will introduce numerical values for the material properties.
The values selected are typical for internal hydrogen as a
solute in AISI 4340 steel.

> Ds:=1e-9;

$$Ds := .1\ 10^{-8}$$

> Vs:=2.02e-6;

$$Vs := .202\ 10^{-5}$$

> traps:=499;

$$traps := 499$$

> c0:=0.0;

$$c0 := 0$$

> MWs:=0.00100797;

$$MWs := .00100797$$

> Em:=200e9;

$$Em := .200\ 10^{12}$$

> nu:=0.3;

$$\nu := .3$$

> rho:=7800;

$$\rho := 7800$$

> T:=293;

$$T := 293$$

> R:=8.31432;

$$R := 8.31432$$

> K;

$$.166666666666667\ 10^{12}$$

> lambda;

$$.115384615384616\ 10^{12}$$

> mu;

$$.769230769230769\ 10^{11}$$

> alpha;

$$5.21047253390476$$

> Rh:=R/MWs;

$$Rh := 8248.57882675080$$

> K1;

$$138.199274509089$$

> K2;

$$7815.70880085715$$

> K1*K2;

$$.108012528605276\ 10^{7}$$

```
> 1/(K1*K2);
```

$$.925818525788271\ 10^{-6}$$

```
> A1;
```

$$.4$$

```
> A2;
```

$$6773.61429407620$$

```
> A3;
```

$$0$$

```
> B1;
```

$$.500000000000001\ 10^{12}$$

```
> B2;
```

$$.390785440042860\ 10^{16}$$

```
> B3;
```

$$0$$

```
Note #6: Now let's solve for the integration constants: _C1, _C2, _C3, and _C4,
         using the boundary data.
```

```
> c2(x);
```

$$_C1$$

```
> _C1:=1e-7;
```

$$_C1 := .1\ 10^{-6}$$

```
> c2(x);
```

$$.1\ 10^{-6}$$

```
> u2(x);
```

$$-.00169340357351905\ x + 2.50000000000000\ x\ _C2 + 1.00000000000000\ _C3$$

```
> eqnset1:={0.0=u2(0.0), 0.0=u2(0.10)};
```

$$eqnset1 := \{\ 0 = 1.00000000000000\ _C3,$$

$$0 = -.000169340357351905 + .250000000000000\ _C2 + 1.00000000000000\ _C3\ \}$$

```
> varset1:={_C2,_C3};
```

$$varset1 := \{\ _C3,\ _C2\ \}$$

```
> solnset1:=solve(eqnset1,varset1);
```

$$solnset1 := \{\ _C3 = 0,\ _C2 = .000677361429407620\ \}$$

```
> assign(solnset1);
```

```
> c2(x);
```

$$.1\ 10^{-6}$$

```
> e2(x);
```

$$.000677361429407620$$

```
> u2(x);
```

$$0$$

```
> S2(x);
```

$$-.521047253390490\ 10^{8}$$

---

1. MAPLE PROGRAM DIRECTORY AND FILE NAME:
/afs/nd.edu/user4/jthomas5/Maple/Transport/1DSSsol#3a.ms

==========

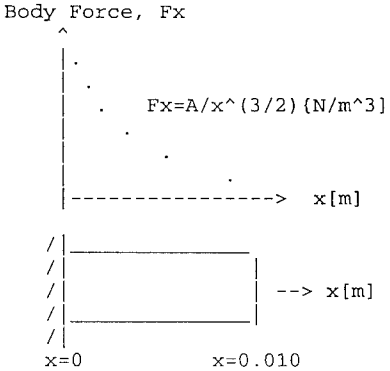
2. ORIGINATOR:
Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637
(219) 631-9371

==========

3. HISTORY:
Written: 12-Nov-1994
Latest Revision: 13-Feb-1995

==========

4. PROGRAM DESCRIPTION:
One-dimensional, steady-state analysis of the fully coupled solute transport and trapping equations using "plane stress" constitutive equations for stress. The particular problem to be solved is shown below. It is the 1-D SS transport problem, but with a (1/x)^(3/2) singular body force applied. This is meant to "simulate" the stress occurring at the tip of a crack:



Deformation variable boundary conditions: u(0)=0, S(0.10)=0
Concentration variable boundary conditions: J(0)=0, c(0.10)=1e-7
Reference concentration level: c0=0.0
Trapping parameter: ltrap=19 (low trapping); htrap=499 (high trapping)
Body Force: A=15x10^6 [N/m^(3/2)]

The equations used in the analysis are:

1. dJ/dx=0 (steady-state diffusion equation)
2. J=Ds*(K1*c*de/dx-dc/dx) (mass flux)
3. dS/dx+Fx=0 (steady-state deformation equation with applied axial body force, Fx)
4. S=B1*e-B2*c+B3 (axial stress)
5. de/dx-K2*dc/dx+Fx/B1=0 (dilational strain gradient)
6. e=A1*du/dx+A2*c-A3 (dilatational strain)

The constants used in the plane stress analysis are defined below:

Ds:=lattice diffusivity [m^2/sec]

K1:=(Vs*K)/(R*T)
Vs:= partial molar volume of solute [m^3/mol solute]
K:= bulk modulus=Em/(3*(1-2*nu)) [N/m^2]
Em:= Modulus of Elasticity [N/m^2]
nu:= Poisson's ratio [1]
R:= universal gas constant=8.31432 [J/mol-K]
T:= temperature [K]

```
B1:=3*K
B2:=9*K*alpha*(1+traps)
B3:=B2*co
(1 or h)traps:= Csr*Kr=trapping constant [1]
Csr:= saturation trap concentration [1]
Kr:= equilibrium trapping constant [1]
c0:= reference solute concentration [1]

K2:=3*alpha*(1+traps)
alpha:= (rho*Vs)/(3*MWs)=solute concentration expansion coefficient [m/m/Delc]
rho:= mass density of the solid [kg/m^3]
MWs:= molecular weight of the solute [kg/mol]
Delc:= c-c0 [1]

A1:=1-2*nu
A2:=2*(1+nu)*alpha*(1+traps)
A3:=A2*c0

======================

5. REQUIRED INPUTS:

Ds:=lattice diffusivity [m^2/sec]
Vs:= partial molar volume of solute [m^3/mol solute]
(1 and h)traps:= Csr*Kr=trapping constant [1]
c0:= reference solute concentration [1]
MWs:= molecular weight of the solute [kg/mol]

Em:= Modulus of Elasticity [Pa]
nu:= Poisson's ratio [1]
rho:= mass density of the solid [kg/m^3]

T:= temperature [K]

======================

6. SYMBOLIC ANALYSIS:
```

```
> restart;
> Digits:=trunc(evalhf(Digits));
```

$$Digits := 15$$

```
> s:=x->B1*e(x)-B2*c(x)+B3;
```

$$s := x \rightarrow B1\ \mathrm{e}(x) - B2\ \mathrm{c}(x) + B3$$

```
> diff(s(x),x)+fx(x);
```

$$B1\left(\frac{\partial}{\partial x}\mathrm{e}(x)\right) - B2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) + \mathrm{fx}(x)$$

```
> dedx:=x->K2*diff(c(x),x)-fx(x)/B1;
```

$$dedx := x \rightarrow K2\ \mathrm{diff}(\mathrm{c}(x), x) - \frac{\mathrm{fx}(x)}{B1}$$

```
> j:=Ds*(K1*c(x)*dedx(x)-diff(c(x),x));
```

$$j := Ds\left(K1\ \mathrm{c}(x)\left(K2\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) - \frac{\mathrm{fx}(x)}{B1}\right) - \left(\frac{\partial}{\partial x}\mathrm{c}(x)\right)\right)$$

```
> J := unapply(Ds*((K1*K2*c(x)-1)*diff(c(x),x)-(K1/B1)*c(x)*F(x)),x);
```

$$J := x \rightarrow Ds\left((K1\ K2\ \mathrm{c}(x) - 1)\ \mathrm{diff}(\mathrm{c}(x), x) - \frac{K1\ \mathrm{c}(x)\ \mathrm{F}(x)}{B1}\right)$$

```
> J(x);
```

$$Ds\left((K1\ K2\ \mathrm{c}(x) - 1)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) - \frac{K1\ \mathrm{c}(x)\ \mathrm{F}(x)}{B1}\right)$$

```
> F:=x->A/x^(3/2);
```

$$F := x \rightarrow \frac{A}{x^{3/2}}$$

```
  Note #1: The governing differential equation in this case is J=constant
           because dJ/dx=0, and we are specifying the value of J(0)=0.
           Setting J(0)=constant produces a DE that is not easily solved.
```

```
> deqn1:=collect(expand(J(x)/(Ds*K1*K2)),diff(c(x),x))=0;
```

$$deqn1 := \left(\mathrm{c}(x) - \frac{1}{K1\ K2}\right)\left(\frac{\partial}{\partial x}\mathrm{c}(x)\right) - \frac{\mathrm{c}(x)\ A}{K2\ B1\ x^{3/2}} = 0$$

```
> soln1:=dsolve(deqn1,c(x));
```

$$soln1 := \mathrm{c}(x) - \frac{\ln(\mathrm{c}(x))}{K1\ K2} + 2\frac{A}{\sqrt{x}\ K2\ B1} = _C1$$

```
  Note #2: We will solve the above equation for c(x) and use this to define a
           new function with {x, A, K2, and _C1} as the argument variables.
```

```
> c:=(x,A,K2,C1)->solve( c-(1/(K1*K2))*ln(c)+(2*A)/(K2*B1*x^(1/2)) = C1,c);
```

$$c := (x, A, K2, C1) \rightarrow \mathrm{solve}\left(c - \frac{\ln(c)}{K1\ K2} + 2\frac{A}{K2\ B1\ \sqrt{x}} = C1, c\right)$$

```
> c(x,A,K2,C1);
```

$$-\frac{\mathrm{W}\left(-K1\ K2\ \mathrm{e}^{\left(\frac{K1\left(2\sqrt{x}\ A - C1\ K2\ B1\ x\right)}{x\ B1}\right)}\right)}{K1\ K2}$$

```
  Note #3a: The above W() function is the "Lambert" function W( ). See the
            Maple help discussion of this function for further details.

  Note #3b: The expression for the classical stress assisted diffusion (SAD)
            concentration is given by setting taking the limit of c(x) as K2->0.
```

```
> csad:=(x,A,C1)->limit(c(x,A,K2,C1),K2=0);
```

$$csad := (x, A, C1) \rightarrow \lim_{K2 \rightarrow 0} \mathrm{c}(x, A, K2, C1)$$

```
> csad(x,A,C1);
```

$$\mathrm{e}^{\left(2\frac{K1\ A}{\sqrt{x}\ B1}\right)}$$

```
> dcdx1:=simplify(diff(c(x,A,K2,C1),x));
```

$$dcdx1 := \frac{\mathrm{W}\left(-K1\ K2\ \mathrm{e}^{\left(\frac{K1\left(2\sqrt{x}\ A - C1\ K2\ B1\ x\right)}{x\ B1}\right)}\right) A}{\left(1 + \mathrm{W}\left(-K1\ K2\ \mathrm{e}^{\left(\frac{K1\left(2\sqrt{x}\ A - C1\ K2\ B1\ x\right)}{x\ B1}\right)}\right)\right) x^{3/2}\ B1\ K2}$$

> diff(W(f(x)),x);

$$\frac{\mathrm{W}(\mathrm{f}(x))\left(\frac{\partial}{\partial x}\mathrm{f}(x)\right)}{(1+\mathrm{W}(\mathrm{f}(x)))\,\mathrm{f}(x)}$$

> int(W(x),x);

$$\mathrm{W}(x)\,x - x + \frac{x}{\mathrm{W}(x)}$$

> x:=(c,A,K2,C1)->solve(c-(1/(K1*K2))*ln(c)+(2*A)/(K2*B1*x^(1/2)) = C1,x);

$$x := (c, A, K2, C1) \rightarrow \mathrm{solve}\left(c - \frac{\ln(c)}{K1\,K2} + 2\,\frac{A}{K2\,B1\,\sqrt{x}} = C1, x\right)$$

> x(c,A,K2,C1);

$$4\,\frac{A^2\,K1^2}{(c\,K1\,K2\,B1 - \ln(c)\,B1 - C1\,K1\,K2\,B1)^2}$$

> dxdc:=(c,A,K2,C1)->diff(x(c,A,K2,C1),c);

$$dxdc := (c, A, K2, C1) \rightarrow \mathrm{diff}(\mathrm{x}(c, A, K2, C1), c)$$

> factor(dxdc(c,A,K2,C1));

$$8\,\frac{A^2\,K1^2\,(c\,K1\,K2 - 1)}{B1^2\,(-c\,K1\,K2 + \ln(c) + C1\,K1\,K2)^3\,c}$$

> factor(1/dxdc(c,A,K2,C1));

$$\frac{1}{8}\,\frac{B1^2\,(-c\,K1\,K2 + \ln(c) + C1\,K1\,K2)^3\,c}{A^2\,K1^2\,(c\,K1\,K2 - 1)}$$

```
Note #4a: dx/dc->0 as c->1/K1*K2, or conversely, dc/dx->infinity as
          c->1/K1*K2! This is apparently a critical point in the
          mathematical solution for the concentration. The concentration
          becomes multivalued at this point.

Note #4b: We will now determine the value of the constant _C1 in terms of
          the concentration at the boundary c(0.1)=cl.
```

> C1:=solve(x(cl,A,K2,C1)=0.1,C1);

$$C1 := -.500000000000000\,\frac{-2.\,B1^2\,cl\,K1^2\,K2^2 + 2.\,B1^2\ln(cl)\,K1\,K2 + 12.6491106406735\,B1\,K1^2\,K2\,A}{B1^2\,K1^2\,K2^2},\ -$$

$$.500000000000000\,\frac{-2.\,B1^2\,cl\,K1^2\,K2^2 + 2.\,B1^2\ln(cl)\,K1\,K2 - 12.6491106406735\,B1\,K1^2\,K2\,A}{B1^2\,K1^2\,K2^2}$$

> C1a:=(cl,A,K2)->expand(-.500000000000000/B1^2/K1^2/K2^2*(-2.*B1^2*cl*K1^2*K2^2+2.*B1^2*ln(cl)*K1*K2+12.6491106406735*B1*K1^2*K2*A));

$$C1a := (cl, A, K2) \rightarrow \mathrm{expand}\left(-.500000000000000\right.$$

$$\frac{-2.\,B1^2\,cl\,K1^2\,K2^2 + 2.\,B1^2\ln(cl)\,K1\,K2 + 12.6491106406735\,B1\,K1^2\,K2\,A}{B1^2\,K1^2\,K2^2}\Bigg)$$

```
> C1b:=(cl,A,K2)->expand( -.500000000000000/B1^2/K1^2/K2^2*(-2.*B1^2*cl*K1^2*K2^2+2.*B1^2*ln(cl)*K1*K2-12.6491106
  406735*B1*K1^2*K2*A));
```

$$C1b := (cl, A, K2) \rightarrow \text{expand}\left(-.500000000000000\right.$$

$$\left.\frac{-2.\,B1^2\,cl\,K1^2\,K2^2 + 2.\,B1^2\ln(cl)\,K1\,K2 - 12.6491106406735\,B1\,K1^2\,K2\,A}{B1^2\,K1^2\,K2^2}\right)$$

```
> C1a(cl,A,K2);
```

$$1.00000000000000\,cl - 1.00000000000000\,\frac{\ln(cl)}{K1\,K2} - 6.32455532033675\,\frac{A}{B1\,K2}$$

```
> C1b(cl,A,K2);
```

$$1.00000000000000\,cl - 1.00000000000000\,\frac{\ln(cl)}{K1\,K2} + 6.32455532033675\,\frac{A}{B1\,K2}$$

```
  Note #5: The quadratic nature of the solution for the constant _C1 yields
           two solutions, C1a & C1b, each of which results in a different
           solution for x(c).
```

```
> xa:=(c,A,K2,cl)->x(c,A,K2,C1a(cl,A,K2));
```

$$xa := (c, A, K2, cl) \rightarrow \mathrm{x}(c, A, K2, \mathrm{C1a}(cl, A, K2))$$

```
> xa(c,A,K2,cl);
```

$$4.\,A^2\,K1^2 \Big/ (c\,K1\,K2\,B1 - 1.\ln(c)\,B1 - 1.00000000000000\,cl\,K1\,K2\,B1$$

$$+ 1.00000000000000\ln(cl)\,B1 + 6.32455532033675\,A\,K1)^2$$

```
> xb:=(c,A,K2,cl)->x(c,A,K2,C1b(cl,A,K2));
```

$$xb := (c, A, K2, cl) \rightarrow \mathrm{x}(c, A, K2, \mathrm{C1b}(cl, A, K2))$$

```
> xb(c,A,K2,cl);
```

$$4.\,A^2\,K1^2 \Big/ (c\,K1\,K2\,B1 - 1.\ln(c)\,B1 - 1.00000000000000\,cl\,K1\,K2\,B1$$

$$+ 1.00000000000000\ln(cl)\,B1 - 6.32455532033675\,A\,K1)^2$$

```
  Note #6: Next we will define the constants, and simplify the two
           concentration expressions for the fully coupled theory and
           classical stress assisted diffusion theory.
```

```
> K:=(Em/(3*(1-2*nu)));
```

$$K := \frac{Em}{3 - 6\,\nu}$$

```
> lambda:=(Em*nu)/((1+nu)*(1-2*nu));
```

$$\lambda := \frac{Em\,\nu}{(1+\nu)(1-2\,\nu)}$$

```
> mu:=Em/(2*(1+nu));
```

$$\mu := \frac{Em}{2 + 2\,\nu}$$

```
> alpha:=(rho*Vs)/(3*MWs);
```

$$\alpha := \frac{1}{3}\,\frac{\rho\ Vs}{MWs}$$

```
> K1:=(Vs*K)/(R*T);
```

$$K1 := \frac{Vs\ Em}{(3 - 6\,\nu)\ R\ T}$$

```
> K2:=3*alpha*(1+traps);
```

$$K2 := \frac{\rho\ Vs\ (1 + traps)}{MWs}$$

```
> A1:=(1-2*nu);
```

$$A1 := 1 - 2\,\nu$$

```
> A2:=2*(1+nu)*alpha*(1+traps);
```

$$A2 := \frac{2}{3}\,\frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)}{MWs}$$

```
> A3:=A2*c0;
```

$$A3 := \frac{2}{3}\,\frac{(1 + \nu)\ \rho\ Vs\ (1 + traps)\ c0}{MWs}$$

```
> B1:=3*K;
```

$$B1 := 3\,\frac{Em}{3 - 6\,\nu}$$

```
> B2:=9*K*alpha*(1+traps);
```

$$B2 := 3\,\frac{Em\ \rho\ Vs\ (1 + traps)}{(3 - 6\,\nu)\ MWs}$$

```
> B3:=B2*c0;
```

$$B3 := 3\,\frac{Em\ \rho\ Vs\ (1 + traps)\ c0}{(3 - 6\,\nu)\ MWs}$$

```
> Ds:=1e-9;
```

$$Ds := .1\ 10^{-8}$$

```
> Vs:=2.02e-6;
```

$$Vs := .202\ 10^{-5}$$

```
> ltraps:=19;
```

$$ltraps := 19$$

```
> htraps:=499;
```

$$htraps := 499$$

```
> c0:=0;
```

$$c0 := 0$$

```
> MWs:=0.00100797;
```

$$MWs := .00100797$$

```
> Em:=200e9;
```

$$Em := .200\ 10^{12}$$

```
> nu:=0.3;
```

$$\nu := .3$$

```
> rho:=7800;
```

$$\rho := 7800$$

```
> T:=293;
```

$$T := 293$$

```
> R:=8.31432;
```

$$R := 8.31432$$

```
> K;
```

$$.166666666666667\ 10^{12}$$

```
> lambda;
```

$$.115384615384616\ 10^{12}$$

```
> mu;
```

$$.769230769230769\ 10^{11}$$

```
> alpha;
```

$$5.21047253390476$$

```
> Rs:=R/MWs;
```

$$Rs := 8248.57882675080$$

```
> K1;
```

$$138.199274509089$$

```
> lK2:=3*alpha*(1+ltraps);
```

$$lK2 := 312.628352034285$$

```
> hK2:=3*alpha*(1+htraps);
```

$$hK2 := 7815.70880085714$$

```
> K1*lK2;
```

$$43205.0114421103$$

```
> 1/(K1*lK2);
```

$$.0000231454631447068$$

```
> K1*hK2;
```

$$.108012528605276\ 10^{7}$$

```
> 1/(K1*hK2);
```

$$.925818525788272\ 10^{-6}$$

```
> A1;
```

$$.4$$

```
> A2;
```

$$13.5472285881524 + 13.5472285881524\ traps$$

```
> A3;
```

$$0$$

```
> B1;
```

$$.500000000000001\ 10^{12}$$

```
> B2;
```

$$.781570880085717\ 10^{13} + .781570880085717\ 10^{13}\ traps$$

```
> B3;
```

$$0$$

Note #7: Concentration for the low trapping situation (i.e., traps=19):

```
> traps:=19;
```

$$traps := 19$$

```
> lA2:=A2;
```

$$lA2 := 270.944571763048$$

```
> lB2:=B2;
```

$$lB2 := .156314176017143\ 10^{15}$$

```
> xal:=(c,A,K2,cl)->xa(c,A,K2,cl);
```

$$xal := xa$$

```
> xal(c,A,K2,cl);
```

$$.163705496009499\ 10^{-27}\ A^2 \Big/ (c - .0000231454631447068 \ln(c) - 1.00000000000001\ cl + .0000231454631447068 \ln(cl) + .404605358354904\ 10^{-13}\ A)^2$$

```
> xbl:=(c,A,K2,cl)->xb(c,A,K2,cl);
```

$$xbl := xb$$

```
> xbl(c,A,K2,cl);
```

$$.163705496009499\ 10^{-27}\ A^2 \Big/ (c - .0000231454631447068 \ln(c) - 1.00000000000001\ cl + .0000231454631447068 \ln(cl) - .404605358354904\ 10^{-13}\ A)^2$$

Note #8: Concentration for the high trapping situation (i.e., traps=499):

```
> traps:=499;
```

$$traps := 499$$

```
> hA2:=A2;
```

$$hA2 := 6773.61429407620$$

```
> hB2:=B2;
```

$$hB2 := .390785440042860\ 10^{16}$$

```
> xah:=(c,A,K2,cl)->xa(c,A,K2,cl);
```

$$xah := xa$$

```
> xah(c,A,K2,cl);
```

$$.261928793615197\ 10^{-30}\ A^2 \Big/ (c - .925818525788271\ 10^{-6} \ln(c) - 1.00000000000001\ cl + .925818525788275\ 10^{-6} \ln(cl) + .161842143341962\ 10^{-14}\ A)^2$$

```
> xbh:=(c,A,K2,cl)->xb(c,A,K2,cl);
```

$$xbh := xb$$

```
> xbh(c,A,K2,cl);
```

$$.261928793615197\ 10^{-30}\ A^2 \Big/ (c - .925818525788271\ 10^{-6} \ln(c) - 1.00000000000001\ cl + .925818525788275\ 10^{-6} \ln(cl) - .161842143341962\ 10^{-14}\ A)^2$$

Note #9: Concentration for SAD:

```
> csad(x,A,cl)->-1.*ln(cl)+.5516800588e-9*A/x^(1/2);
```

$$\mathrm{csad}(x, A, cl) \rightarrow -1.\ln(cl) + .5516800588\ 10^{-9} \frac{A}{\sqrt{x}}$$

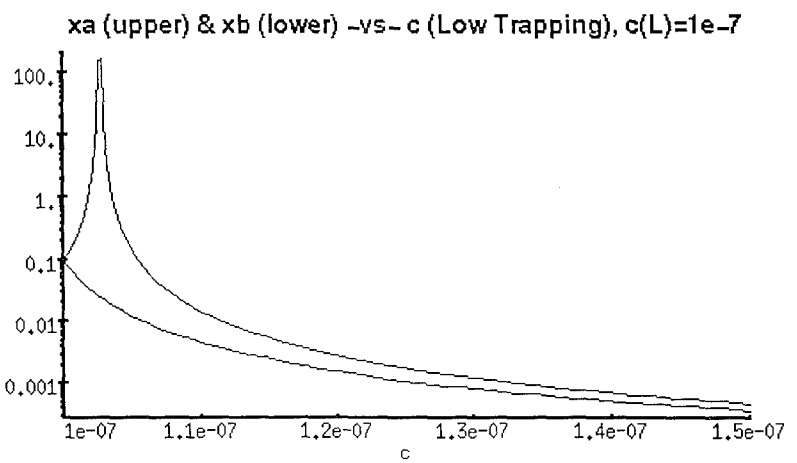
```
> Csad1(x,A,cl);
```

$$\mathrm{Csad1}(x, A, cl)$$

```
> with(plots);
```

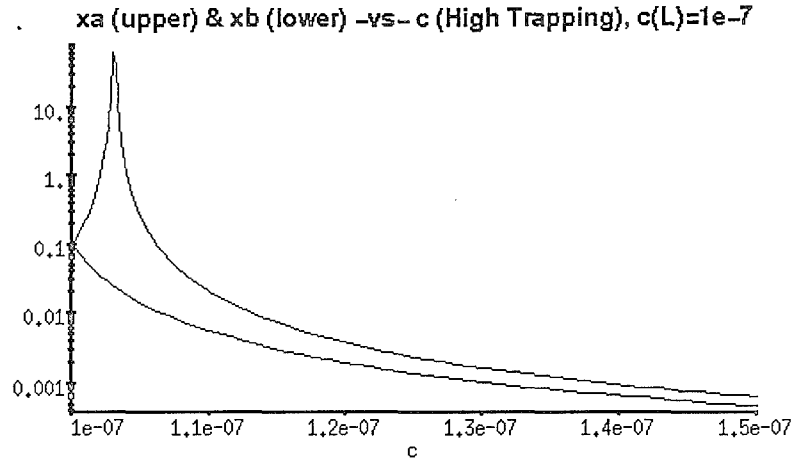
[*animate*, *animate3d*, *conformal*, *contourplot*, *cylinderplot*, *densityplot*, *display*, *display3d*, *fieldplot*, *fieldplot3d*, *gradplot*, *gradplot3d*, *implicitplot*, *implicitplot3d*, *loglogplot*, *logplot*, *matrixplot*, *odeplot*, *pointplot*, *polarplot*, *polygonplot*, *polygonplot3d*, *polyhedraplot*, *replot*, *setoptions*, *setoptions3d*, *spacecurve*, *sparsematrixplot*, *sphereplot*, *surfdata*, *textplot*, *textplot3d*, *tubeplot*]

```
>
> logplot({xal(c,15e6,lK2,1e-7),
> xbl(c,15e6,lK2,1e-7)},c=1e-7..1.5e-7,
> title='xa (upper) & xb (lower) -vs- c (Low Trapping), c(L)=1e-7');
>
```



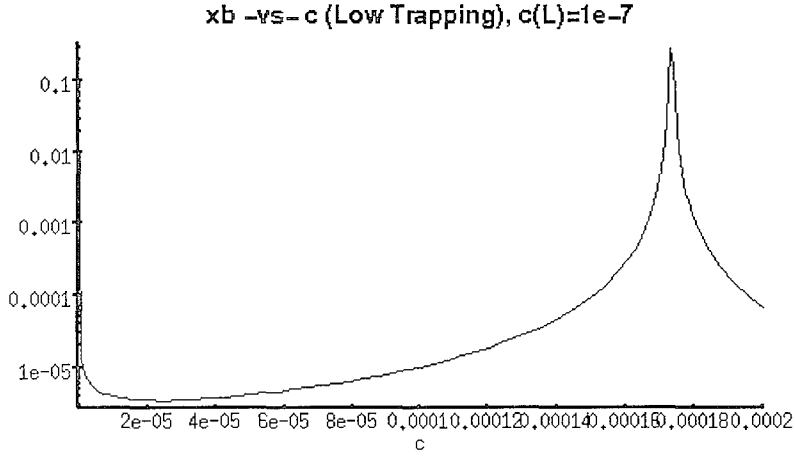

```
>
>
> logplot({xah(c,15e6,hK2,1e-7),
> xbh(c,15e6,hK2,1e-7)},c=1e-7..1.5e-7,
```

```
> title='xa (upper) & xb (lower) -vs- c (High Trapping), c(L)=1e-7');
>
```

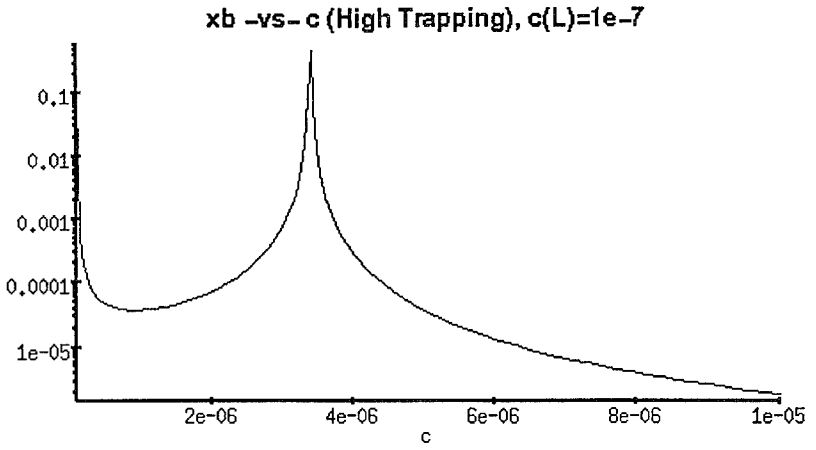


Note #11: The above plots show that the C1b parameter is clearly correct for c(L)=1e-7. The xa(c) solution predicts a singularity at the minimum concentration level on the rod, which is of no physical use. We must now determine, however, whether the xb(c) solution is valid for all c if c(L)=1e-7.

```
> logplot(xbl(c,15e6,lK2,1e-7),
> c=1e-7..2e-4,title='xb -vs- c (Low Trapping), c(L)=1e-7');
>
```




```
>
> logplot(xbh(c,15e6,hK2,1e-7),
> c=1e-7..1e-5,title='xb -vs- c (High Trapping), c(L)=1e-7');
>
```



Note #12a: THE ABOVE PLOTS DO NOT HAVE THE SAME CONCENTRATION AXES. While the second plot appears to show that the singularity shifts toward a higher concentration level, this is only caused by a change in the axis scaling -- the singularity shift is toward lower concentration levels.

Note #12b: Both xa(c) & xb(c) become multi-valued at some critical value of c which is dependent on the level of trapping present in the model, but independent of the left-hand concentration. We must determine the value of x where this critical value of concentration occurs as x decreases from L=0.1 to 0.0.

```
> cbl_cr:=solve(diff(xbl(c,15e6,IK2,cl),c)=0,c);
```

$$cbl_cr := .0000231454631447068$$

```
> xblmin:=xbl(cbl_cr,15e6,IK2,1e-9);
```

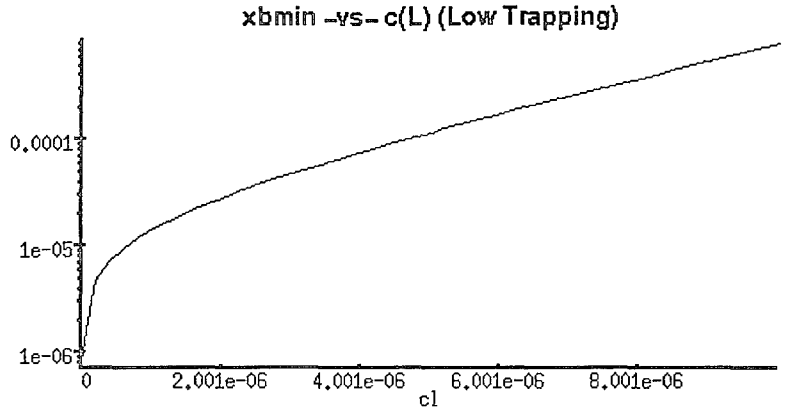
$$xblmin := .834723037961544\ 10^{-6}$$

```
> xblmin:=xbl(cbl_cr,15e6,IK2,1e-7);
```

$$xblmin := .343354181482430\ 10^{-5}$$

Note #13: The limit concentration is independent of c(L), but the value of x(c) which corresponds to this limit concentration is obviously highly dependent on c(L). We now examine the nature of this dependence.

```
> logplot(xbl(cbl_cr,15e6,IK2,cl),cl=1e-9..1e-5,title='xbmin -vs- c(L) (Low Trapping)');
>
```



>
> cbh_cr:=solve(diff(xbh(c,15e6,hK2,cl),c)=0,c);

$$cbh_cr := .925818525788272\ 10^{-6}$$

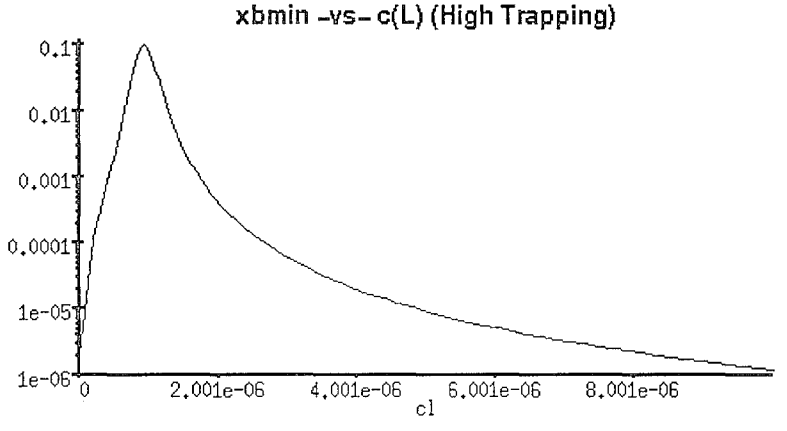
> xbhmin:=xbh(cbh_cr,15e6,hK2,1e-9);

$$xbhmin := .200363349240182\ 10^{-5}$$

> xbhmin:=xbh(cbh_cr,15e6,hK2,1e-7);

$$xbhmin := .0000371878414183777$$

> logplot(xbh(cbh_cr,15e6,hK2,cl),cl=1e-9..1e-5,title='xbmin -vs- c(L) (High Trapping)');
>

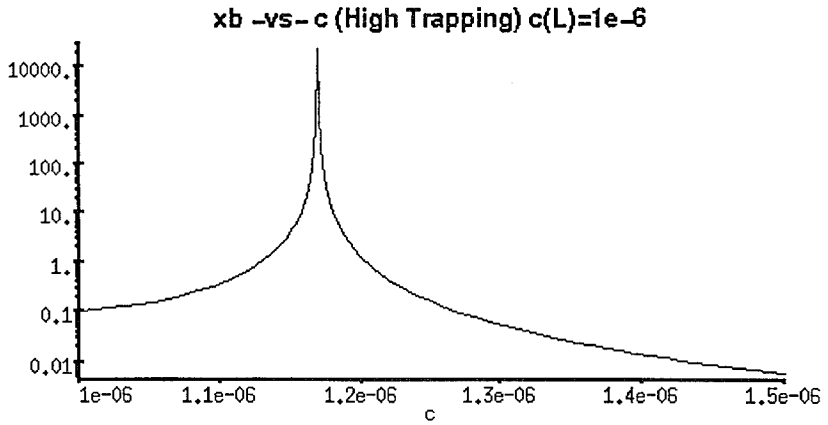


Note #14: The threshold level of c(L) at which xb(c) is no longer valid and xa(c) becomes the physically meaningful solution may also be determined.

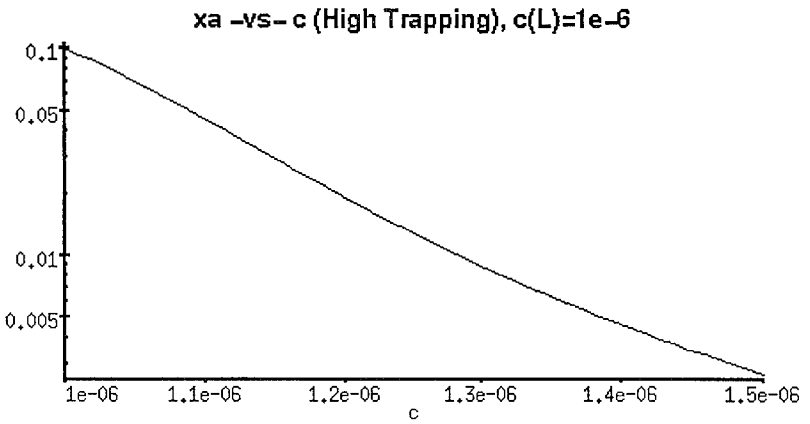
> solve(diff(xbh(cbh_cr,15e6,hK2,cl),cl)=0,cl);

$$.925818525788271\ 10^{-6}$$

> logplot(xbh(c,15e6,hK2,1e-6),c=1e-6..1.5e-6,title='xb -vs- c (High Trapping) c(L)=1e-6');
>



> logplot(xah(c,15e6,hK2,1e-6),c=1e-6..1.5e-6,title='xa -vs- c (High Trapping), c(L)=1e-6');
>



Note #15a: The solution is divided, then, into two regimes. The first,with c(L)<c(L)critical, requires the xb solution, while the second, with c(L)>c(L)critical, requries the xa solution. The exact value of c(L)critical is dependent on the level of trapping present in the problem.

Note #15b: To directly compare the concentration predictions generated by variations in trapping and c(L), we define new concentration functions.

> cb:=(x,A,K2,cl)->c(x,A,K2,C1b(cl,A,K2));

$$cb := (x, A, K2, cl) \rightarrow \mathrm{c}(x, A, K2, \mathrm{C1b}(cl, A, K2))$$

> cb(x,A,lK2,cl);

$$-.0000231454631447068\ \mathrm{W}\left(-43205.0114421103\ e^{\left(-.432050114421103\ 10^{-23}\right.}\right.$$
$$\left.\left(.404605358354905\ 10^{15}\ A\ x - .231454631447069\ 10^{24}\ \ln(cl)\ x + .100000000000000\ 10^{29}\ cl\ x - .127947448591013\ 10^{15}\ \sqrt{x\ A}\right)/x\right)\Big)$$

> K2:='K2';

$$K2 := K2$$

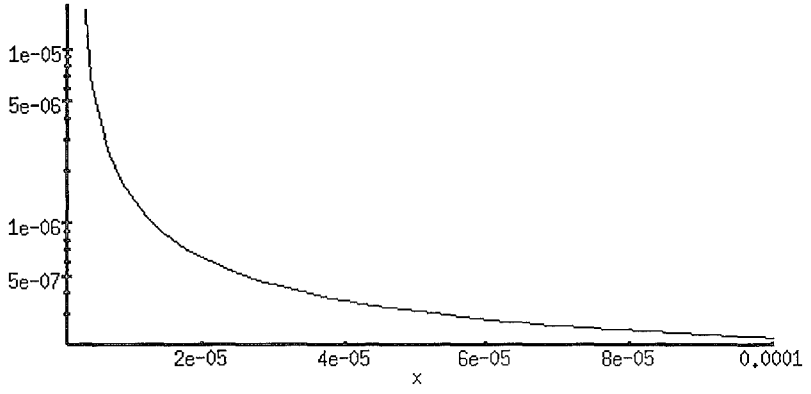
> csad1:=(x,A,cl)->csad(x,A,C1b(cl,A,K2));

$$csad1 := (x, A, cl) \rightarrow \mathrm{csad}(x, A, \mathrm{C1b}(cl, A, K2))$$

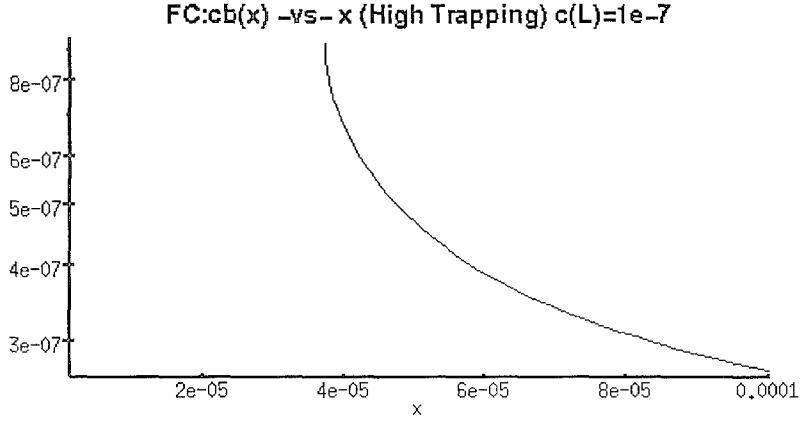
> simplify(expand(csad1(x,A,cl)));

$$cl^{\frac{125000000000001298170446072 71}{125000000000000000000000000000}} e^{\left(-.221118839214542\ 10^{-21}\ \frac{A\left(.7905694150421\ 10^{13}\sqrt{x}-.2500000000000\ 10^{13}\right)}{\sqrt{x}}\right)}$$

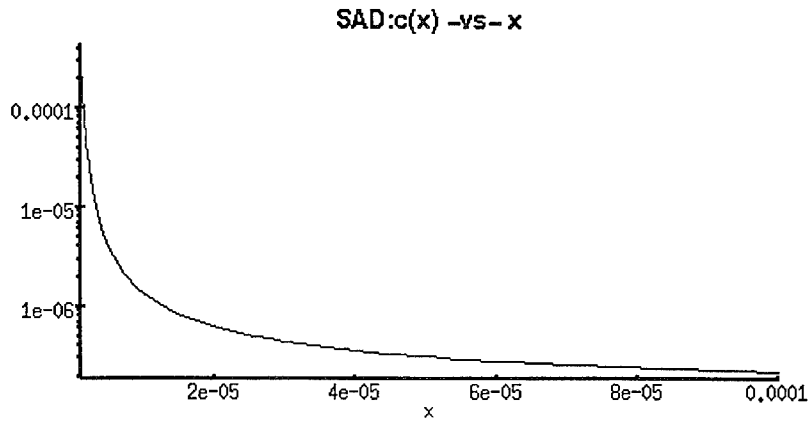
```
> p4:=logplot(cb(x,15e6,lK2,1e-7),x=1e-6..1e-4,title='FC:cb(x) -vs- x (Low Trapping) c(L)=1e-7'):
> p4;
>
```



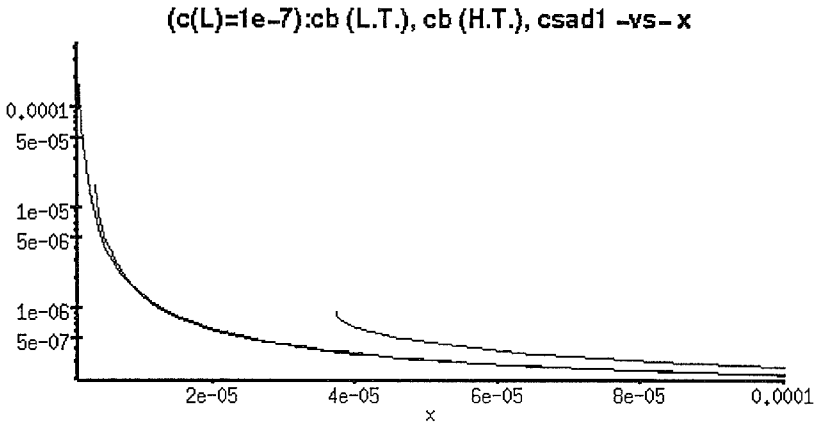

```
> p5:=logplot(cb(x,15e6,hK2,1e-7),x=1e-6..1e-4,resolution=100000,
> title='FC:cb(x) -vs- x (High Trapping) c(L)=1e-7'):
> p5;
>
```




```
> p6:=logplot(csad1(x,15e6,1e-7),x=1e-6..1e-4,
> resolution=10000,title='SAD:c(x) -vs- x'):
> p6;
>
```

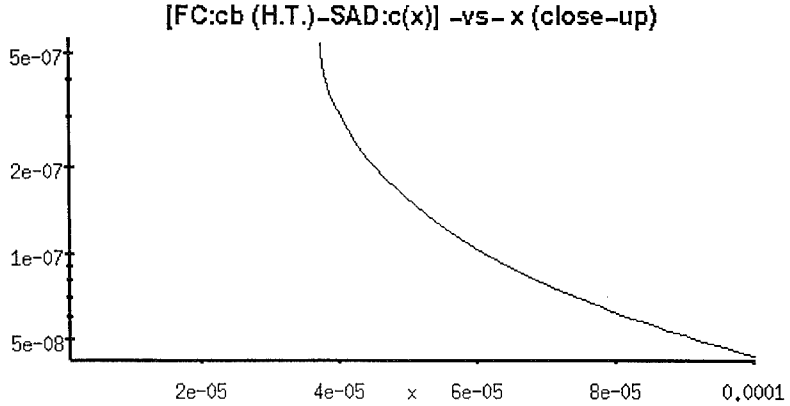



```
> display([p4,p5,p6],title='(c(L)=1e-7):cb (L.T.), cb (H.T.), csad1 -vs- x');
>
```

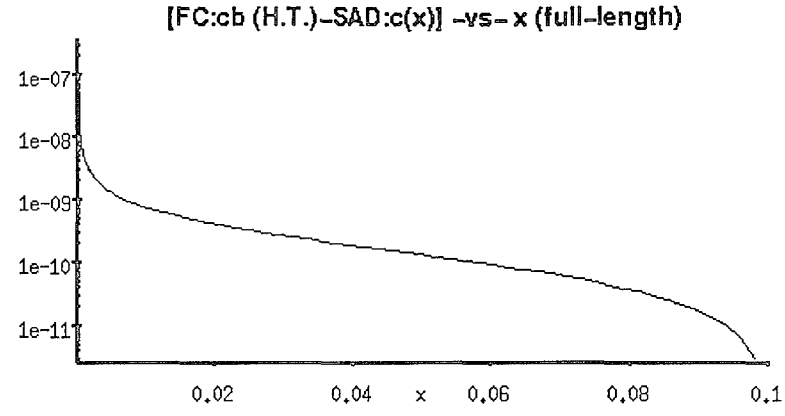


Note #16: The above plots indicate that the difference between SAD and Fully Coupled hydrogen concentration is strongly dependent on the degree of trapping.

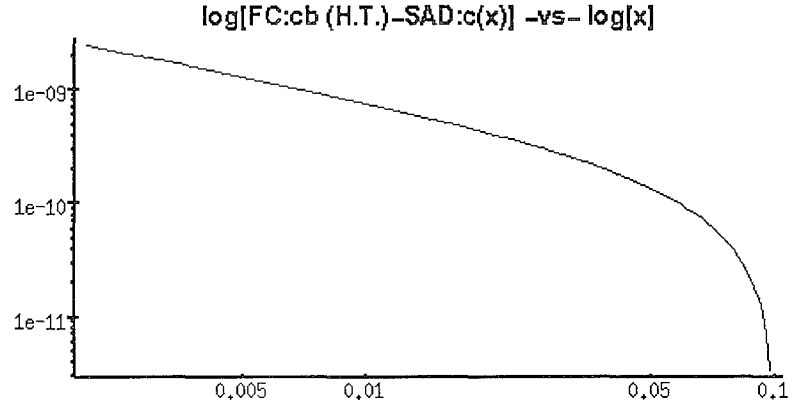
```
> logplot(cb(x,15e6,hK2,1e-7)-csad1(x,15e6,1e-7),x=1e-6..1e-4,
> resolution=10000,title='[FC:cb (H.T.)-SAD:c(x)] -vs- x (close-up)') ;
>
```




```
>
> logplot(cb(x,15e6,hK2,1e-7)-csad1(x,15e6,1e-7),x=1e-6..1e-1,
> resolution=10000,title='[FC:cb (H.T.)-SAD:c(x)] -vs- x (full-length)') ;
>
```




```
>
> loglogplot([x,cb(x,15e6,hK2,1e-7)-csad1(x,15e6,1e-7),x=1e-6..1e-1],
> resolution=10000,title='log[FC:cb (H.T.)-SAD:c(x)] -vs- log[x]');
>
```



```
  Note #17a: Calculate the stress, strain and displacements:

  Note #17b: Stress is calculated by integration of the body force with the
             boundary condition that the right end of the rod is stress
             free.
```

```
> int(-A/x^(3/2),x);
```

$$2\frac{A}{\sqrt{x}}$$

```
> C2:=(x,A)->-(2*A)/x^(1/2);
```

$$C2 := (x, A) \rightarrow -2\frac{A}{\sqrt{x}}$$

```
> C2(0.1,15e6);
```

$$-.948683298050514\ 10^{8}$$

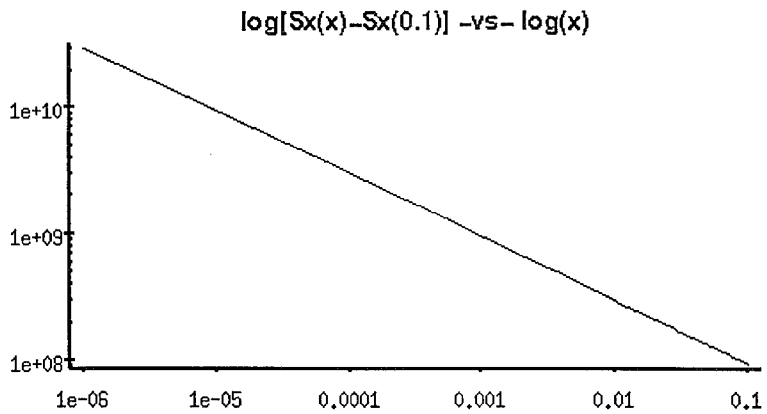
```
> Sx:=(x)->(2*15e6)/x^(1/2)+C2(0.1,15e6);
```

$$Sx := x \rightarrow .30\ 10^{8}\frac{1}{\sqrt{x}} + C2(.1, .15\ 10^{8})$$

```
> Sx(x);
```

$$.30\ 10^{8}\ \frac{1}{\sqrt{x}} - .948683298050514\ 10^{8}$$

```
> loglogplot([x,(Sx(x)-C2(0.1,15e6)),x=1e-6..0.1],title='log[Sx(x)-Sx(0.1)] -vs- log(x)');
>
```



```
Note #18: Strain is calculated from the constitutive relationship, Eq.(4).
          Without displacements due to concentration, strain may be
          calculated from the standard linear-elastic constitutive
          relationship for comparison.
```

```
> eh:=x->Sx(x)/(3*K)+3*alpha*500*cb(x,15e6,hK2,1e-7);
```

$$eh := x \rightarrow \frac{1}{3}\frac{\mathrm{Sx}(x)}{K} + 1500\ \alpha\ \mathrm{cb}(x, .15\ 10^{8}, hK2, .1\ 10^{-6})$$

```
> eh(x);
```

$$.0000599999999999999\ \frac{1}{\sqrt{x}} - .000189736659610102 - .00723592799999999$$

$$\mathrm{W}\left(-.108012528605276\ 10^{7}\ e^{\left(\frac{-.200903303205813\ 10^{-14}\ .808962789010000\ 10^{16}\ x\ -\ .4127337051323\ 10^{13}\ \sqrt{x}}{x}\right)}\right)$$

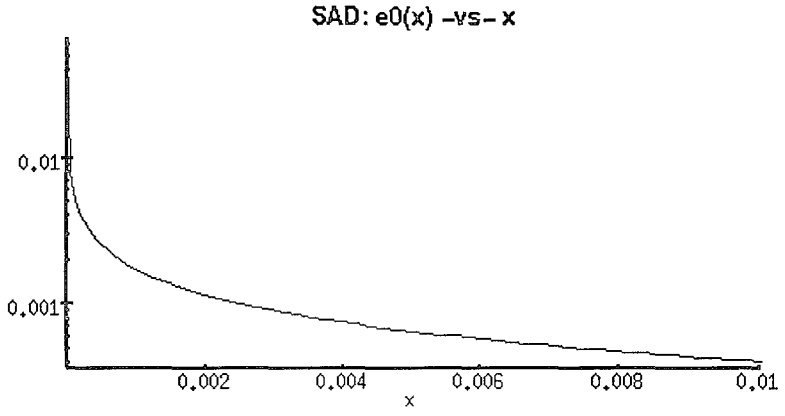
```
> e0:=x->Sx(x)/(3*K);
```

$$e0 := x \rightarrow \frac{1}{3}\frac{\mathrm{Sx}(x)}{K}$$

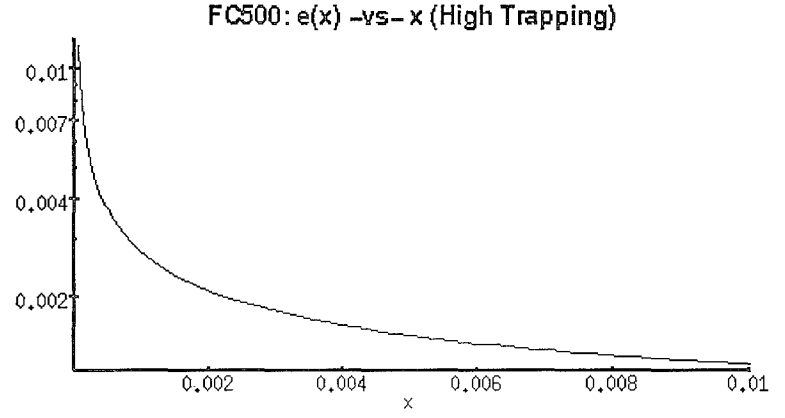
```
> e0(x);
```

$$.0000599999999999999\ \frac{1}{\sqrt{x}} - .000189736659610102$$

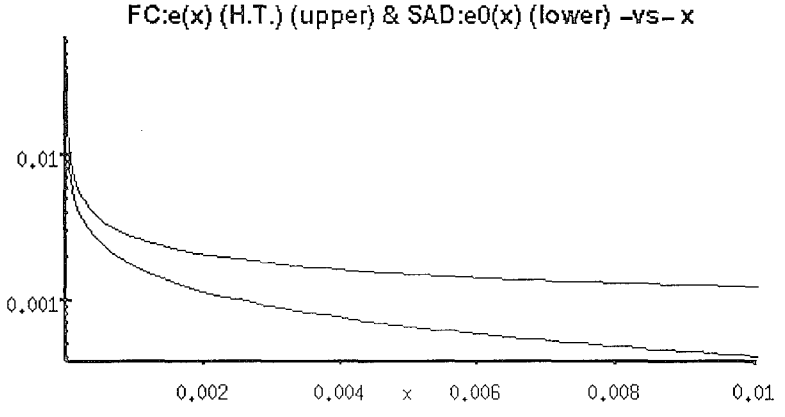
```
> p7:=logplot(e0(x),x=1e-6..0.01,title='SAD: e0(x) -vs- x'):
> p7;
>
```



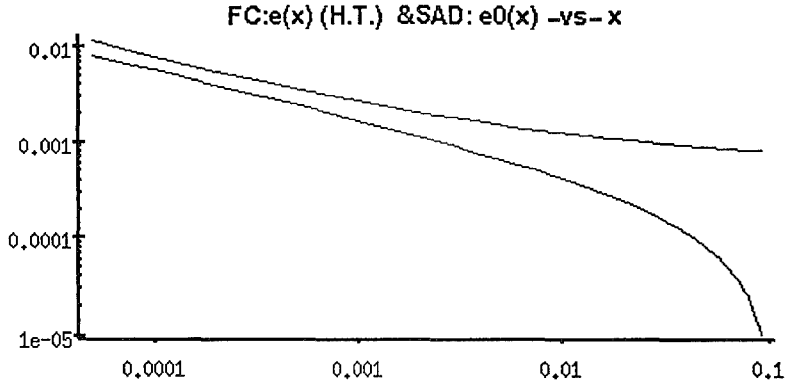

```
> p8:=logplot(eh(x),x=1e-6..0.01,title='FC500: e(x) -vs- x (High Trapping)'):
> p8;
>
```



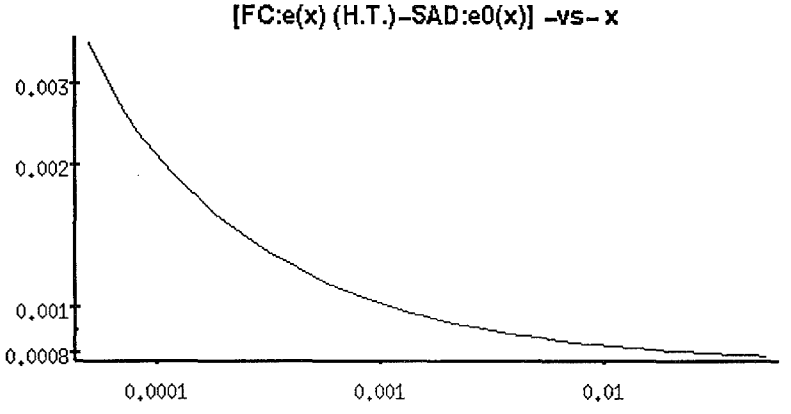

```
> display([p7,p8],title='FC:e(x) (H.T.) (upper) & SAD:e0(x) (lower) -vs- x');
>
```




```
> p9:=loglogplot([x,e0(x),x=5e-5..0.09]):
> p9;
> p10:=loglogplot([x,eh(x),x=5e-5..0.09]):
> p10;
> display([p9,p10], title='FC:e(x) (H.T.)  &SAD: e0(x) -vs- x');
>
```




```
> loglogplot([x,eh(x)-e0(x),x=5e-5..0.09],title='[FC:e(x) (H.T.)-SAD:e0(x)] -vs- x');
>
```



```
  Note #19: Axial displacement is calculated by integrating the
            strain-displacement relation Eq.(6) over the length of the rod.
```

```
> ux:=x->(15e6/Em)*(4*sqrt(x)-6.32456*x)+alpha*500*
> int(c(x,15e6,hK2,C1b(1e-7,15e6,hK2)),x=0..'x');
```

$$ux := x \rightarrow .15\ 10^{8}\ \frac{4\ \mathrm{sqrt}(x) - 6.32456\ x}{Em} + 500\ \alpha\ \mathrm{int}(\mathrm{c}(x, .15\ 10^{8}, hK2, \mathrm{C1b}(.1\ 10^{-6}, .15\ 10^{8}, hK2)), x = 0\ ..\ 'x')$$

```
> ux(x);
```

$$.000300000000000000\ \sqrt{x} - .000474342000000000\ x + 2605.23626695238 \int_{0}^{x} - .925818525788272\ 10^{-6}\ \mathrm{W}\left(-.108012528605276\ 10^{7}\ \mathrm{e}^{\left(-.200903303205813\ 10^{-14}\ \frac{.808962789010000\ 10^{16}\ x - .4127337051323\ 10^{13}\ \sqrt{x}}{x}\right)}\right) dx$$

APPENDIX B: User Element Subroutine

This Appendix contains a copy of the Fortran user element subroutine for solving fully coupled deformation-diffusion problems in one-dimension. A listing of the subroutine is given first, and is followed by an annotated listing.

NOTE: This User Element Subroutine is used with ABAQUS Standard, Version 5.3.1, and is run on a Sun SPARC 10 workstation with the following software configuration: SUN OS 4.1.3; FORTRAN level V2.0.1; C level SC2.0.1 (libansi.a © Sun Microsystems, Inc.); X Windows level X11 Release 4.

DISCLAIMER: *This ABAQUS "user element" subroutine is provided free of charge as a courtesy to the technical community. The authors and the University of Notre Dame accept no responsibility for any decisions based upon the use of this subroutine. Each user is advised that the subroutine has been tested against a limited number of steady-state deformation-diffusion problems, and has been found to give accurate answers to these particular test problems. The accuracy of this subroutine cannot be guaranteed in any particular future analysis.*

Developer Contact:

Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637

Phone: (219) 631- 9371
Fax: (219) 631-8341
e-Mail: James.P.Thomas.66@nd.edu

ABAQUS User Element Subroutine for Coupled Deformation-Diffusion Problems: Fortran 77 Code

```
      subroutine UEL(RHS,AMATRX,SVARS,ENERGY,NDOFEL,NRHS,NSVARS,PROPS,
     1 NPROPS,COORDS,MCRD,NNODE,U,DU,V,A,JTYPE,TIME,DTIME,KSTEP,KINC,
     2 JELEM,PARAMS,NDLOAD,JDLTYP,ADLMAG,PREDEF,NPREDF,LFLAGS,
     3 MLVARX,DDLMAG,MDLOAD,PNEWDT)
C
      include 'ABA_PARAM.INC'
C     implicit double precision (A-H,O-Z) <= input from included program
C
      dimension RHS(MLVARX,*),AMATRX(NDOFEL,NDOFEL),SVARS(NSVARS),
     1 ENERGY(8),PROPS(*),COORDS(MCRD,NNODE),
     2 U(NDOFEL),DU(MLVARX,*),V(NDOFEL),A(NDOFEL),TIME(2),
     3 PARAMS(3),JDLTYP(MDLOAD,*),ADLMAG(MDLOAD,*),
     4 DDLMAG(MDLOAD,*),PREDEF(NPREDF,NNODE,2),LFLAGS(4)
C
      double precision AREA,XNU,BULK,ALPHA,D,XKON1,FUN,
     1 FNU(2),F(2),CREF,RHO,XMW,TEMP,RS,GW(2),GR(2),E,A1,A2,A3,
     2 B1,B2,B3,XJI(2),DJ(2),X(3),XGAUS(2),XKC(2,2),XKU(3,3),
     3 XKUC(3,2),CAP(2,2),E1,E2,DE,R(5),DEFF,TRAPS

      integer KFLAG

      double precision XJAC,DETJ,G1,G2,DG1,DG2,H1,H2,H3,DH1,DH2,DH3
      external XJAC,DETJ,G1,G2,DG1,DG2,H1,H2,H3,DH1,DH2,DH3

C
C     ******************************************************************
C     * 1-D, 3-NODE ISOPARAMETRIC DISPLACEMENT/2-NODE SUPERPARAMETRIC  *
C     * CONCENTRATION USER ELEMENT FOR MUTUALLY COUPLED                *
C     * STATIC/TRANSIENT STRESS-ASSISTED DIFFUSION PROBLEMS            *
C     * (CONSTANT CROSS-SECTIONAL AREA)                                *
C     *                                                                *
C     * /|                                                             *
C     * /|  Node:  1               2               3                  *
C     * /|---------*===============*===============*-------> x,u       *
C     * /|  Pos:   x1------L/2-----x2------L/2-----x3                  *
C     * /|  Conc:  c1                              c2                 *
C     * /|  Disp:  u1              u2              u3                 *
C     *                                                                *
C     *                                                                *
C     *               SOLUTION DEPENDENT STATE VARIABLES               *
C     *    SVARS(1)= DILATATIONAL STRAIN AT INTEGRATION POINT GR(1) [1] *
C     *    SVARS(2)= DILATATIONAL STRAIN AT INTEGRATION POINT GR(2) [1] *
C     *    SVARS(3)= AXIAL STRESS AT INTEGRATION POINT GR(1)       [Pa] *
C     *    SVARS(4)= AXIAL STRESS AT INTEGRATION POINT GR(2)       [Pa] *
C     *    SVARS(5)= AXIAL STRESS AT LEFT END OF ELEMENT           [Pa] *
C     *    SVARS(6)= AXIAL STRESS AT RIGHT END OF ELEMENT          [Pa] *
C     *    SVARS(7)= MASS FLUX AT THE CENTER OF EACH ELEMENT     [m/s] *
C     *    SVARS(8)= X LOCATION OF INTEGRATION POINT GR(1)         [m] *
C     *    SVARS(9)= X LOCATION OF INTEGRATION POINT GR(2)         [m] *
C     *                                                                *
C     *                                                                *
C     *         BASED ON THEORY AND EQUATIONS BY DR. JAMES P. THOMAS   *
C     *         CODED BY CHARLES E. P. CHOPIN, 25 AUGUST 1994          *
C     *         LAST MODIFIED BY CHARLES E. P. CHOPIN,  13 MARCH 1995  *
C     *         DEPARTMENT OF AEROSPACE AND MECHANICAL ENGINEERING     *
C     *         UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA          *
C     *                                                                *
C     *         DIRECT INQUIRIES REGARDING THIS USER ELEMENT           *
C     *         SUBROUTINE TO:                                         *
C     *                   James.P.Thomas.66@nd.edu                     *
C     *                                                                *
C     ******************************************************************
C
C       DEGREES OF FREEDOM FOR MODEL IN ORDER:
C              {C1,U1,U2,C2,U3}'
C
C       C      =       NODAL MASS FRACTION CONCENTRATION OF
C                        SOLUTE                    [kgSOLUTE/kgSOLID]
C       U      =       NODAL DISPLACEMENT                        [m]
C       KFLAG  =       CASE FLAG FOR PLANE STRESS OR PLANE STRAIN [1]
C       AREA   =       CROSS-SECTIONAL AREA OF THE ROD         [m^2]
```

```
C       E       =       YOUNG'S MODULUS FOR THE SOLID                [Pa]
C       XNU     =       POISSON'S RATIO FOR THE SOLID                 [1]
C       D       =       DIFFUSION COEFFICIENT FOR SOLUTE IN SOLID [m^2/s]
C       ALPHA   =       SOLUTE EXPANSION COEFFICIENT                  [1]
C                       =(1/3)*(RHO*(PARTIAL MOLAR VOLUME OF SOLUTE))/XMW
C       CREF    =       REFERENCE CONCENTRATION        [kgSOLUTE/kgSOLID]
C       RHO     =       DENSITY OF SOLID MIXTURE                 [kg/m^3]
C       XMW     =       MOLECULAR WEIGHT FOR SOLUTE SPECIES      [kg/mol]
C       TEMP    =       AMBIENT TEMPERATURE (ASSUMED CONSTANT)        [K]
C       TRAPS   =       TRAP SITES CONSTANT (CSRKR IN (1+CSRKR) TERM) [1]
C
      KFLAG  =int(PROPS(1))
      AREA   =PROPS(2)
      E      =PROPS(3)
      XNU    =PROPS(4)
      D      =PROPS(5)
      ALPHA  =PROPS(6)
      CREF   =PROPS(7)
      RHO    =PROPS(8)
      XMW    =PROPS(9)
      TEMP   =PROPS(10)
      TRAPS  =PROPS(11)

C       2-POINT GAUSSIAN INTEGRATION LOCATIONS AND WEIGHTS
C
     data GR/-0.577350269189626D0,0.577350269189626D0/,
     1     GW/ 1.000000000000000D0,1.000000000000000D0/

C
C       RS      =       GAS CONSTANT FOR SOLUTE SPECIES
C       BULK    =       BULK MODULUS FOR THE SOLID
C       XKON1   =       NON-DIMENSIONAL COEFFICIENT FOR (C*DE/DX) TERM OF
C                       MASS FLUX EQUATION
C                       (J=-DEFF*DC/DX + DEFF*XKON1*C*DE/DX)
C       DEFF    =       EFFECTIVE DIFFUSION COEFFICIENT
C
      RS     = 8.31432D0/XMW
      BULK   = E/(3.0D0*(1.0D0-2.0D0*XNU))
      XKON1  = 3.0D0*BULK*ALPHA/(RHO*RS*TEMP)
      DEFF   = D/(1.0D0+TRAPS )

C
C       SET CONSTANTS FOR PLANE STRESS OR PLANE STRAIN CASE
C       1=> PLANE STRESS, FULLY COUPLED
C       2=> PLANE STRAIN, FULLY COUPLED
C       3=> PLANE STRESS, WEAKLY COUPLED
C       4=> PLANE STRAIN, WEAKLY COUPLED
C
      if(KFLAG.eq.1) then
            A1=(1.0D0-2.0D0*XNU)
            A2=(2.0D0*(1.0D0+XNU)*ALPHA)*(1.0D0+TRAPS)
            A3=(A2*CREF)
            B1=(3.0D0*BULK)
            B2=(9.0D0*BULK*ALPHA)*(1.0D0+TRAPS)
            B3=(B2*CREF)
      elseif(KFLAG.eq.2) then
            A1=1.0D0
            A2=0.0D0
            A3=0.0D0
            B1=(1.0D0-XNU)*E/((1.0D0+XNU)*(1.0D0-2.0D0*XNU))
            B2=(3.0D0*BULK*ALPHA)*(1.0D0+TRAPS)
            B3=(B2*CREF)
      elseif(KFLAG.eq.3) then
            A1=(1.0D0-2.0D0*XNU)
            A2=0.0D0
            A3=0.0D0
            B1=(3.0D0*BULK)
            B2=0.0D0
            B3=0.0D0
      elseif(KFLAG.eq.4) then
            A1=1.0D0
            A2=0.0D0
            A3=0.0D0
            B1=(1.0D0-XNU)*E/((1.0D0+XNU)*(1.0D0-2.0D0*XNU))
            B2=0.0D0
            B3=0.0D0
```

```
      endif
C
C       SET X COORDINATES FOR NODES ON CURRENT ELEMENT
C
        X(1)=COORDS(1,1)+U(2)
        X(2)=COORDS(1,2)+U(3)
        X(3)=COORDS(1,3)+U(5)
C
C       SET GLOBAL COORDINATES FOR GAUSS POINTS ON CURRENT ELEMENT
C
        XGAUS(1)=H1(GR(1))*X(1)+H2(GR(1))*X(2)+H3(GR(1))*X(3)
        XGAUS(2)=H1(GR(2))*X(1)+H2(GR(2))*X(2)+H3(GR(2))*X(3)
C
C       CALCULATE INVERSE JACOBIAN AND DETERMINANT FOR ISOPARAMETRIC
C       TRANSFORMATION
C
        do 20 I = 1,2
           XJI(I)=1.0D0/XJAC(GR(I),X(1),X(2),X(3))
           DJ(I)=DETJ(GR(I),X(1),X(2),X(3))
 20     continue

        if(LFLAGS(1).ne.71)then
C
C       <<<<<<<<<<<  CALCULATE CAPACITANCE MATRIX >>>>>>>>>
C
      CAP(1,1)   = AREA*(G1(GR(1))*G1(GR(1))*DJ(1)*GW(1)
     1             + G1(GR(2))*G1(GR(2))*DJ(2)*GW(2))

      CAP(1,2)   = AREA*(G1(GR(1))*G2(GR(1))*DJ(1)*GW(1)
     1             + G1(GR(2))*G2(GR(2))*DJ(2)*GW(2))

      CAP(2,1)   = AREA*(G2(GR(1))*G1(GR(1))*DJ(1)*GW(1)
     1             + G2(GR(2))*G1(GR(2))*DJ(2)*GW(2))

      CAP(2,2)   = AREA*(G2(GR(1))*G2(GR(1))*DJ(1)*GW(1)
     1             + G2(GR(2))*G2(GR(2))*DJ(2)*GW(2))
      endif
C
C
C       <<<<<<<<<<<  CALCULATE STIFFNESS MATRICES >>>>>>>>>
C
C       CALCULATE de/dr FROM PREVIOUS TIME STEP FOR NON-LINEAR TERM
C
      E1=SVARS(1)
      E2=SVARS(2)
      DE = (E2-E1)/(GR(2)-GR(1))
C
C       COEFFICIENTS OF CONCENTRATION D.O.F. IN MASS BALANCE EQUATION
C
     XKC(1,1)  = AREA*DEFF*(XJI(1)*(DG1(GR(1))*DG1(GR(1))
     1             -XKON1*DG1(GR(1))*DE*G1(GR(1)))*GW(1)
     2                +XJI(2)*(DG1(GR(2))*DG1(GR(2))
     3             -XKON1*DG1(GR(2))*DE*G1(GR(2)))*GW(2))

     XKC(1,2)  = AREA*DEFF*(XJI(1)*(DG1(GR(1))*DG2(GR(1))
     1             -XKON1*DG1(GR(1))*DE*G2(GR(1)))*GW(1)
     2               + XJI(2)*(DG1(GR(2))*DG2(GR(2))
     3             -XKON1*DG1(GR(2))*DE*G2(GR(2)))*GW(2))

     XKC(2,1)  = AREA*DEFF*(XJI(1)*(DG2(GR(1))*DG1(GR(1))
     1             -XKON1*DG2(GR(1))*DE*G1(GR(1)))*GW(1)
     2               + XJI(2)*(DG2(GR(2))*DG1(GR(2))
     3             -XKON1*DG2(GR(2))*DE*G1(GR(2)))*GW(2))

     XKC(2,2)  = AREA*DEFF*(XJI(1)*(DG2(GR(1))*DG2(GR(1))
     1             -XKON1*DG2(GR(1))*DE*G2(GR(1)))*GW(1)
     2               + XJI(2)*(DG2(GR(2))*DG2(GR(2))
     3             -XKON1*DG2(GR(2))*DE*G2(GR(2)))*GW(2))
C
C
C       COEFFICIENTS OF CONCENTRATION IN LINEAR MOMENTUM BALANCE EQUATION
C
     XKUC(1,1) = AREA*(B1*A2-B2)*((DH1(GR(1))*G1(GR(1)))*GW(1)
     1                    + (DH1(GR(2))*G1(GR(2)))*GW(2))
```

```
      XKUC(1,2) = AREA*(B1*A2-B2)*((DH1(GR(1))*G2(GR(1)))*GW(1)
     1                     + (DH1(GR(2))*G2(GR(2)))*GW(2))

      XKUC(2,1) = AREA*(B1*A2-B2)*((DH2(GR(1))*G1(GR(1)))*GW(1)
     1                     + (DH2(GR(2))*G1(GR(2)))*GW(2))

      XKUC(2,2) = AREA*(B1*A2-B2)*((DH2(GR(1))*G2(GR(1)))*GW(1)
     1                     + (DH2(GR(2))*G2(GR(2)))*GW(2))

      XKUC(3,1) = AREA*(B1*A2-B2)*((DH3(GR(1))*G1(GR(1)))*GW(1)
     1                     + (DH3(GR(2))*G1(GR(2)))*GW(2))

      XKUC(3,2) = AREA*(B1*A2-B2)*((DH3(GR(1))*G2(GR(1)))*GW(1)
     1                     + (DH3(GR(2))*G2(GR(2)))*GW(2))
C
C
C       COEFFICIENTS OF DISPLACEMENT IN LINEAR MOMENTUM BALANCE EQUATION
C
      XKU(1,1)  = AREA*B1*A1*(XJI(1)*(DH1(GR(1))*DH1(GR(1)))*GW(1)
     1                + XJI(2)*(DH1(GR(2))*DH1(GR(2)))*GW(2))

      XKU(1,2)  = AREA*B1*A1*(XJI(1)*(DH1(GR(1))*DH2(GR(1)))*GW(1)
     1                + XJI(2)*(DH1(GR(2))*DH2(GR(2)))*GW(2))

      XKU(1,3)  = AREA*B1*A1*(XJI(1)*(DH1(GR(1))*DH3(GR(1)))*GW(1)
     1                + XJI(2)*(DH1(GR(2))*DH3(GR(2)))*GW(2))

      XKU(2,1)  = AREA*B1*A1*(XJI(1)*(DH2(GR(1))*DH1(GR(1)))*GW(1)
     1                + XJI(2)*(DH2(GR(2))*DH1(GR(2)))*GW(2))

      XKU(2,2)  = AREA*B1*A1*(XJI(1)*(DH2(GR(1))*DH2(GR(1)))*GW(1)
     1                + XJI(2)*(DH2(GR(2))*DH2(GR(2)))*GW(2))

      XKU(2,3)  = AREA*B1*A1*(XJI(1)*(DH2(GR(1))*DH3(GR(1)))*GW(1)
     1                + XJI(2)*(DH2(GR(2))*DH3(GR(2)))*GW(2))

      XKU(3,1)  = AREA*B1*A1*(XJI(1)*(DH3(GR(1))*DH1(GR(1)))*GW(1)
     1                + XJI(2)*(DH3(GR(2))*DH1(GR(2)))*GW(2))

      XKU(3,2)  = AREA*B1*A1*(XJI(1)*(DH3(GR(1))*DH2(GR(1)))*GW(1)
     1                 + XJI(2)*(DH3(GR(2))*DH2(GR(2)))*GW(2))

      XKU(3,3)  = AREA*B1*A1*(XJI(1)*(DH3(GR(1))*DH3(GR(1)))*GW(1)
     1                 + XJI(2)*(DH3(GR(2))*DH3(GR(2)))*GW(2))
C
C
        if(LFLAGS(1).eq.71) then
C
C               *******************************
C        ************* STEADY STATE DIFFUSION *******************
C               *******************************

        if (LFLAGS(3).eq.1.or.LFLAGS(3).eq.2) then
C
C         <<<<<< CALCULATE AMATRX = [K] >>>>>>>>>>>>
C         WHERE [K] IS
C               [XKC(1,1)  0       0       XKC(1,2)  0       ]
C               [XKUC(1,1) XKU(1,1) XKU(1,2) XKUC(1,2) XKU(1,3)]
C               [XKUC(2,1) XKU(2,1) XKU(2,2) XKUC(2,2) XKU(2,3)]
C               [XKC(2,1)  0       0       XKC(2,2)  0       ]
C               [XKUC(3,1) XKU(3,1) XKU(3,2) XKUC(3,2) XKU(3,3)]


        AMATRX(1,1) = XKC(1,1)
        AMATRX(1,4) = XKC(1,2)
        AMATRX(2,1) = XKUC(1,1)
        AMATRX(2,2) = XKU(1,1)
        AMATRX(2,3) = XKU(1,2)
        AMATRX(2,4) = XKUC(1,2)
        AMATRX(2,5) = XKU(1,3)
        AMATRX(3,1) = XKUC(2,1)
        AMATRX(3,2) = XKU(2,1)
        AMATRX(3,3) = XKU(2,2)
        AMATRX(3,4) = XKUC(2,2)
        AMATRX(3,5) = XKU(2,3)
        AMATRX(4,1) = XKC(2,1)
```

```
      AMATRX(4,4) = XKC(2,2)
      AMATRX(5,1) = XKUC(3,1)
      AMATRX(5,2) = XKU(3,1)
      AMATRX(5,3) = XKU(3,2)
      AMATRX(5,4) = XKUC(3,2)
      AMATRX(5,5) = XKU(3,3)

      endif
C
      if((LFLAGS(3).eq.1).or.(LFLAGS(3).eq.5)) then
C
C
C      <<<<<< CALCULATE {RHS} = {R}-[K]{U} >>>>>>>>>>>>
C       NB:  THIS USER ELEMENT ASSUMES THAT ALL OF THE
C            NEUMANN BOUNDARY DATA ARE HOMOGENEOUS (i.e., ZERO).
C            INHOMOGENEOUS (NON-ZERO) NEUMANN BOUNDARY DATA SUCH
C            AS NON-ZERO BOUNDARY TRACTIONS AND/OR SOLUTE FLUXES
C            ARE AUTOMATICALLY INCORPORATED INTO THE COMPUTATIONS
C            BY ABAQUS.  INHOMOGENEOUS DATA SHOULD BE ENTERED IN
C            THE INPUT DECK AS CONCENTRATED NODAL FORCES.
C
C     THE FOLLOWING SECTION CALCULATES THE TOTAL USER SPECIFIED
C     DISTRIBUTED LOADS (e.g. BODY FORCES) AT THE GAUSS POINTS
C     ON THE ROD FOR USE IN FINDING THE RHS VECTOR.
C
     FUN=0.0D0
      do 31 I=1,2
         F(I) = 0.0D0
         FNU(I) = 0.0D0
 31   continue
      do 41 K1=1,MDLOAD
           if(JDLTYP(K1,1).gt.0)then
               FUN=FUN+ADLMAG(K1,1)
           elseif(JDLTYP(K1,1).lt.0)then
               call KFCALC(JDLTYP(K1,1),F,XGAUS,TIME(2))
               do 51 I=1,2
                  FNU(I)=FNU(I)+F(I)
 51            continue
           endif
 41    continue
       do 61 I=1,2
          FNU(I)=FNU(I)+FUN
 61    continue
C
C
C
      R(1) = 0.0D0
C
      R(2)= AREA*((H1(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH1(GR(1)))*DJ(1)*GW(1)
     2       +(H1(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH1(GR(2)))*DJ(2)*GW(2))
C
      R(3)= AREA*((H2(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH2(GR(1)))*DJ(1)*GW(1)
     2       +(H2(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH2(GR(2)))*DJ(2)*GW(2))
C
      R(4) = 0.0D0
C
      R(5)= AREA*((H3(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH3(GR(1)))*DJ(1)*GW(1)
     2       +(H3(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH3(GR(2)))*DJ(2)*GW(2))
C
      RHS(1,1) = R(1) -XKC(1,1)*U(1)-XKC(1,2)*U(4)
C
      RHS(2,1) = R(2) -XKUC(1,1)*U(1)-XKU(1,1)*U(2)-XKU(1,2)*U(3)
     1                -XKUC(1,2)*U(4)-XKU(1,3)*U(5)
C
      RHS(3,1) = R(3) -XKUC(2,1)*U(1)-XKU(2,1)*U(2)-XKU(2,2)*U(3)
     1                -XKUC(2,2)*U(4)-XKU(2,3)*U(5)
C
      RHS(4,1) = R(4) -XKC(2,1)*U(1)-XKC(2,2)*U(4)
C
      RHS(5,1) = R(5) -XKUC(3,1)*U(1)-XKU(3,1)*U(2)-XKU(3,2)*U(3)
```

```
     1                -XKUC(3,2)*U(4)-XKU(3,3)*U(5)
C
C
       endif

      elseif((LFLAGS(1).eq.72).or.(LFLAGS(1).eq.73)) then
C
C             ******************************
C       ************* TRANSIENT DIFFUSION ******************
C             ******************************
C
      if (LFLAGS(3).eq.1.or.LFLAGS(3).eq.2) then
C
C        <<<<<< CALCULATE AMATRX = [[K]+[C]/DTIME] >>>>>>>>>>>>
C        WHERE [K] IS
C              [XKC(1,1)  0       0       XKC(1,2)  0      ]
C              [XKUC(1,1) XKU(1,1) XKU(1,2) XKUC(1,2) XKU(1,3)]
C              [XKUC(2,1) XKU(2,1) XKU(2,2) XKUC(2,2) XKU(2,3)]
C              [XKC(2,1)  0       0       XKC(2,2)  0      ]
C              [XKUC(3,1) XKU(3,1) XKU(3,2) XKUC(3,2) XKU(3,3)]
C
C
C        AND [C] IS
C              [CAP(1,1) 0       0       CAP(1,2) 0]
C              [0        0       0       0        0]
C              [0        0       0       0        0]
C              [CAP(2,1) 0       0       CAP(2,2) 0]
C              [0        0       0       0        0]
C
C
      AMATRX(1,1) = XKC(1,1) + CAP(1,1)/DTIME
      AMATRX(1,4) = XKC(1,2) + CAP(1,2)/DTIME
      AMATRX(2,1) = XKUC(1,1)
      AMATRX(2,2) = XKU(1,1)
      AMATRX(2,3) = XKU(1,2)
      AMATRX(2,4) = XKUC(1,2)
      AMATRX(2,5) = XKU(1,3)
      AMATRX(3,1) = XKUC(2,1)
      AMATRX(3,2) = XKU(2,1)
      AMATRX(3,3) = XKU(2,2)
      AMATRX(3,4) = XKUC(2,2)
      AMATRX(3,5) = XKU(2,3)
      AMATRX(4,1) = XKC(2,1) + CAP(2,1)/DTIME
      AMATRX(4,4) = XKC(2,2) + CAP(2,2)/DTIME
      AMATRX(5,1) = XKUC(3,1)
      AMATRX(5,2) = XKU(3,1)
      AMATRX(5,3) = XKU(3,2)
      AMATRX(5,4) = XKUC(3,2)
      AMATRX(5,5) = XKU(3,3)

      endif
C
C
C
      if((LFLAGS(3).eq.1).or.(LFLAGS(3).eq.5)) then
C
C       <<<<<< CALCULATE {RHS} = {R}-[K]{U}-([C]/DTIME){DU}>>>>>>
C
C      THE FOLLOWING SECTION CALCULATES THE TOTAL USER SPECIFIED
C      DISTRIBUTED LOADS (e.g. BODY FORCES) AT THE GAUSS POINTS
C      ON THE ROD FOR USE IN FINDING THE RHS VECTOR.
C
      FUN=0.0D0
       do 131 I=1,2
          F(I) = 0.0D0
          FNU(I) = 0.0D0
 131   continue
       do 141 K1=1,MDLOAD
            if(JDLTYP(K1,1).gt.0)then
                FUN=FUN+ADLMAG(K1,1)
            elseif(JDLTYP(K1,1).lt.0)then
                call KFCALC(JDLTYP(K1,1),F,XGAUS,TIME(2))
                do 151 I=1,2
                   FNU(I)=FNU(I)+F(I)
 151            continue
            endif
```

```
 141    continue
        do 161 I=1,2
           FNU(I)=FNU(I)+FUN
 161    continue
C
C
C
       R(1) = 0.0D0
C
       R(2)= AREA*((H1(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH1(GR(1)))*DJ(1)*GW(1)
     2       +(H1(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH1(GR(2)))*DJ(2)*GW(2))
C
       R(3)= AREA*((H2(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH2(GR(1)))*DJ(1)*GW(1)
     2       +(H2(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH2(GR(2)))*DJ(2)*GW(2))
C
       R(4) = 0.0D0
C
       R(5)= AREA*((H3(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH3(GR(1)))*DJ(1)*GW(1)
     2       +(H3(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH3(GR(2)))*DJ(2)*GW(2))
C
C
       RHS(1,1) = R(1) -XKC(1,1)*U(1)-XKC(1,2)*U(4)
     1                 -1.0D0/DTIME*(CAP(1,1)*DU(1,1)+CAP(1,2)*DU(4,1))
C
       RHS(2,1) = R(2) -XKUC(1,1)*U(1)-XKU(1,1)*U(2)-XKU(1,2)*U(3)
     1                 -XKUC(1,2)*U(4)-XKU(1,3)*U(5)
C
       RHS(3,1) = R(3) -XKUC(2,1)*U(1)-XKU(2,1)*U(2)-XKU(2,2)*U(3)
     1                 -XKUC(2,2)*U(4)-XKU(2,3)*U(5)
C
       RHS(4,1) = R(4) -XKC(2,1)*U(1)-XKC(2,2)*U(4)
     1                 -1.0D0/DTIME*(CAP(2,1)*DU(1,1)+CAP(2,2)*DU(4,1))
C
       RHS(5,1) = R(5) -XKUC(3,1)*U(1)-XKU(3,1)*U(2)-XKU(3,2)*U(3)
     1                 -XKUC(3,2)*U(4)-XKU(3,3)*U(5)
C
C
       endif
C
C     <<<<<< CHECK THAT PROCEDURE FLAG SENT MATCHES PROCEDURE PERFORMED >>>
C
      elseif((LFLAGS(1).ne.71).and.
     1    (LFLAGS(1).ne.72).and.(LFLAGS(1).ne.73)) then
       write(*,*) 'ERROR IN THE VALUE OF LFLAGS(1) = ',LFLAGS(1)
         endif
C
       if(LFLAGS(3).eq.1) then
C
C      <<<<<<<<<<<  CALCULATE STRESSES AND STRAINS AT THE GAUSS POINTS >>>
C
C         DILATATIONAL STRAINS:
          SVARS(1) =  A1*XJI(1)*(DH1(GR(1))*U(2)
     1                        +DH2(GR(1))*U(3)+DH3(GR(1))*U(5))
     2               +A2*(G1(GR(1))*U(1)+G2(GR(1))*U(4))-A3
          SVARS(2) =  A1*XJI(2)*(DH1(GR(2))*U(2)+
     1                         DH2(GR(2))*U(3)+DH3(GR(2))*U(5))
     2               +A2*(G1(GR(2))*U(1)+G2(GR(2))*U(4))-A3


C         GAUSS POINT STRESSES:
          SVARS(3) = B1*SVARS(1)-B2*(G1(GR(1))*U(1)+G2(GR(1))*U(4))+B3
          SVARS(4) = B1*SVARS(2)-B2*(G1(GR(2))*U(1)+G2(GR(2))*U(4))+B3

C         OUTER NODE STRESSES:
          DE = (SVARS(2)-SVARS(1))/(GR(2)-GR(1))
          SVARS(5) = B1*(SVARS(1)+(-1.0D0-GR(1))*DE)-B2*U(1)+B3
          SVARS(6) = B1*(SVARS(2)+( 1.0D0-GR(2))*DE)-B2*U(4)+B3

C         CENTROIDAL SOLUTE MASS FLUX
          SVARS(7)=D*(1.0D0/XJAC(0.0D0,X(1),X(2),X(3)))
```

```
     1           *(-(DG1(0.0D0)*U(1)+DG2(0.0D0)*U(4))+
     2             XKON1*(G1(0.0D0)*U(1)+G2(0.0D0)*U(4))*DE)

C       GLOBAL GAUSS POINTS LOCATIONS
          SVARS(8)=XGAUS(1)
          SVARS(9)=XGAUS(2)
C
C
        endif
        return
        end
C
C
C       **********************************************
C
C
        double precision function XJAC(R,X1,X2,X3)
        double precision R,X1,X2,X3
C       CALCULATE JACOBIAN OF ISOPARAMETRIC TRANSFORMATION
C           (D/DR=XJAC^(-1)*D/DX)
              XJAC=(R-1.0D0/2.0D0)*X1-2.0D0*R*X2+(R+1.0D0/2.0D0)*X3
        return
        end
C
C
C
C
        double precision function DETJ(R,X1,X2,X3)
        double precision R,X1,X2,X3
C       CALCULATE DETERMINANT OF JACOBIAN OF ISOPARAMETRIC TRANSFORMATION
C       (DR=DETJ*DX)
             DETJ=(R-1.0D0/2.0D0)*X1-2.0D0*R*X2+(R+1.0D0/2.0D0)*X3
        return
        end
C
C
C
C       LINEAR INTERPOLATION FUNCTIONS FOR CONCENTRATION
C
        double precision function G1(R)
        double precision R
              G1=(1.0D0/2.0D0)*(1.0D0-R)
        return
        end
C
C
        double precision function G2(R)
        double precision R
              G2=(1.0D0/2.0D0)*(1.0D0+R)
        return
        end
C
C
C
C        QUADRATIC INTERPOLATION FUNCTIONS FOR DISPLACEMENT
C
        double precision function H1(R)
        double precision R
              H1=1.0D0/2.0D0*(R**2-R)
        return
        end
C
C
        double precision function H2(R)
        double precision R
              H2=1.0D0-R**2
        return
        end
C
C
        double precision function H3(R)
        double precision R
              H3=1.0D0/2.0D0*(R**2+R)
        return
        end
C
```

```
C
C
C     DERIVATIVES OF LINEAR INTERPOLATIONS FOR CONCENTRATION
C
      double precision function DG1(R)
      double precision R
            DG1=(-1.0D0/2.0D0)
      return
      end
C
C
      double precision function DG2(R)
      double precision R
            DG2=(1.0D0/2.0D0)
      return
      end
C
C
C
C     DERIVATIVES OF QUADRATIC INTERPOLATIONS FOR DISPLACEMENT
C
      double precision function DH1(R)
      double precision R
            DH1=(R-1.0D0/2.0D0)
      return
      end
C
C
      double precision function DH2(R)
      double precision R
            DH2=-2.0D0*R
      return
      end
C
C
      double precision function DH3(R)
      double precision R
            DH3=(R+1.0D0/2.0D0)
      return
      end
C
C
C
C     DISTRIBUTED LOAD SPECIFICATION ROUTINE
C
      subroutine KFCALC(JDLTYP,F,XGAUS,TTIME)
      double precision F(*),XGAUS(*),TTIME
      integer JDLTYP,I

      double precision A,EPS
C     THIS LOAD ROUTINE CALCULATES THE BODY FORCE AT THE
C     GAUSS POINTS FOR USE IN FINDING THE RHS VECTOR

      IF(JDLTYP.EQ.-1) THEN
C
C        LOAD TYPE 1 INDICATES A DISTRIBUTED BODY FORCE OF THE FORM
C           F(X)= A/(X+EPS)^3/2
C        GRAVITATIONAL BODY FORCE FOR 4340 STEEL IS ~80.0D3 [N/m^3]
C        'A' SHOULD BE SPECIFIED IN UNITS OF [FORCE/LENGTH^3/2]

         A=15.0D6
         EPS=1.0D-18


        DO 100 I=1,2
  100   F(I)=A/sqrt((abs(XGAUS(I))+EPS)**3.0D0)


      ENDIF


      return
      end
```

ABAQUS User Element Subroutine for Coupled Deformation-Diffusion Problems: Annotated Description

DISCLAIMER

This ABAQUS "user element" subroutine is provided free of charge as a courtesy to the technical community. The authors and the University of Notre Dame accept no responsibility for any decisions based upon the use of this subroutine. Each user is advised that the subroutine has been tested against a limited number of steady-state deformation-diffusion problems, and has been found to give accurate answers to these particular test problems. The accuracy of this subroutine cannot be guaranteed in any particular future analysis.

Format of the Coding Notes

The left hand side of the page contains the actual Fortran coding of the ABAQUS User Element subroutine and the right hand side of the page contains explanations of the coding and assumptions, and justifications for certain coding techniques. Blank lines have been added to the subroutine in this listing for ease of readability.

This one-dimensional subroutine is primarily intended as a stepping-stone to a two-dimensional subroutine. A clear understanding of the one-dimensional formulation, which uses 5×5 capacitance and stiffness matrices, will help simplify the task of understanding the corresponding two-dimensional model which requires 20×20 matrices.

The notes on the right side of the page are intended to be as complete as is possible without repeating the comments already in the code. Familiarity with the standard ABAQUS user element variables is assumed. Additional information concerning these variables can be found in the ABAQUS User's Manual (Book II; Section 5.2.16). All further references to the ABAQUS User's Manual will be denoted by AUM.

All major steps in the Fortran code are indicated in the notes by beginning the line in **BOLD, UNDERLINED, AND CAPITALIZED** type. An attempt has been made to refer to all Fortran variables in `COURIER CAPITALS` and any variables which relate directly to the analysis and derivation of this code in *variable script*.

Description of the Subroutine

This "User Element" subroutine is useful for analyzing steady-state and transient one-dimensional deformation-diffusion problems. By changing certain parameters in the ABAQUS input deck, the user may choose between plane-stress or plane-strain constitutive behavior, and fully-coupled, weakly-coupled (Stress Assisted Diffusion), or uncoupled behavior of the solute-solid system.

Developer Contact:

Dr. James P. Thomas
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637

Phone: (219) 631- 9371
Fax: (219) 631-8341
e-Mail: James.P.Thomas.66@nd.edu

```
      subroutine UEL(RHS,AMATRX,SVARS,ENERGY,NDOFEL,NRHS,NSVARS,PROPS,
     1 NPROPS,COORDS,MCRD,NNODE,U,DU,V,A,JTYPE,TIME,DTIME,KSTEP,KINC,
     2 JELEM,PARAMS,NDLOAD,JDLTYP,ADLMAG,PREDEF,NPREDF,LFLAGS,
     3 MLVARX,DDLMAG,MDLOAD,PNEWDT)
C
        include 'ABA_PARAM.INC'
C        implicit double precision (A-H,O-Z) <= input from included program
C
```

The initial subroutine declaration, include statement, and dimension statement are provided in the AUM (II; 5.2.16-1). These three statements are the same for all User Elements. ABAQUS uses implicit type definition of variables. The program `'ABA_PARAM.INC'` specifies whether the implicit variables are `REAL` or `DOUBLE PRECISION` based on the configuration of the computer used in the analysis.

```
       dimension RHS(MLVARX,*),AMATRX(NDOFEL,NDOFEL),SVARS(NSVARS),
     1 ENERGY(8),PROPS(*),COORDS(MCRD,NNODE),
     2 U(NDOFEL),DU(MLVARX,*),V(NDOFEL),A(NDOFEL),TIME(2),
     3 PARAMS(3),JDLTYP(MDLOAD,*),ADLMAG(MDLOAD,*),
     4 DDLMAG(MDLOAD,*),PREDEF(NPREDF,NNODE,2),LFLAGS(4)
C
       double precision AREA,XNU,BULK,ALPHA,D,XKON1,FUN,
     1 FNU(2),F(2),CREF,RHO,XMW,TEMP,RS,GW(2),GR(2),E,A1,A2,A3,
     2 B1,B2,B3,XJI(2),DJ(2),X(3),XGAUS(2),XKC(2,2),XKU(3,3),
     3 XKUC(3,2),CAP(2,2),E1,E2,DE,R(5),DEFF,TRAPS

       integer KFLAG

       double precision XJAC,DETJ,G1,G2,DG1,DG2,H1,H2,H3,DH1,DH2,DH3
       external XJAC,DETJ,G1,G2,DG1,DG2,H1,H2,H3,DH1,DH2,DH3
```

DECLARE all local double precision variables.

DECLARE all local double precision arrays.

DECLARE functions used by `subroutine UEL` as double precision.
EXTERNAL FUNCTIONS are defined and used by `subroutine UEL`.

NOTE: ABAQUS uses implicit declaration of variables to simplify the transition between computers using double and single precision variable defaults. All local variables in this routine are explicitly declared `double precision`, but the variables are named to take advantage of ABAQUS implicit declarations found in `'ABA_PARAM.INC'` should this be necessary or desired.

```
C
C     ************************************************************************
C     * 1-D, 3-NODE ISOPARAMETRIC DISPLACEMENT/2-NODE SUPERPARAMETRIC        *
C     * CONCENTRATION USER ELEMENT FOR MUTUALLY COUPLED                      *
C     * STATIC/TRANSIENT STRESS-ASSISTED DIFFUSION PROBLEMS                  *
C     * (CONSTANT CROSS-SECTIONAL AREA)                                      *
C     *                                                                      *
C     * /|                                                                  *
C     * /|  Node:  1               2               3                       *
C     * /|---------*===============*===============*-------> x,u            *
C     * /|   Pos:   x1------L/2-----x2------L/2-----x3                       *
C     * /|   Conc:  c1                              c2                      *
C     * /|   Disp:  u1              u2              u3                      *
C     *                                                                      *
C     *                                                                      *
C     *               SOLUTION DEPENDENT STATE VARIABLES                     *
C     *    SVARS(1)= DILATATIONAL STRAIN AT INTEGRATION POINT GR(1) [1]      *
C     *    SVARS(2)= DILATATIONAL STRAIN AT INTEGRATION POINT GR(2) [1]      *
C     *    SVARS(3)= AXIAL STRESS AT INTEGRATION POINT GR(1)       [Pa]      *
C     *    SVARS(4)= AXIAL STRESS AT INTEGRATION POINT GR(2)       [Pa]      *
C     *    SVARS(5)= AXIAL STRESS AT LEFT END OF ELEMENT           [Pa]      *
C     *    SVARS(6)= AXIAL STRESS AT RIGHT END OF ELEMENT          [Pa]      *
C     *    SVARS(7)= MASS FLUX AT THE CENTER OF EACH ELEMENT      [m/s]      *
C     *    SVARS(8)= X LOCATION OF INTEGRATION POINT GR(1)          [m]      *
C     *    SVARS(9)= X LOCATION OF INTEGRATION POINT GR(2)          [m]      *
C     *                                                                      *
C     *         BASED ON THEORY AND EQUATIONS BY DR. JAMES P. THOMAS         *
C     *         CODED BY CHARLES E. P. CHOPIN, 25 AUGUST 1994                *
C     *         LAST MODIFIED BY CHARLES E. P. CHOPIN, 13 MARCH 1995         *
C     *         DEPARTMENT OF AEROSPACE AND MECHANICAL ENGINEERING           *
C     *         UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA                *
C     *                                                                      *
C     *         DIRECT E-MAIL INQUIRIES REGARDING THIS USER ELEMENT          *
C     *         SUBROUTINE TO:                                               *
C     *                    James.P. Thomas66@nd.edu                          *
C     *                                                                      *
C     ************************************************************************
```

The user element has three nodes. Concentration degrees-of-freedom (dof) are assigned at the two outer nodes, and axial displacement dof are assigned at all three nodes. An isoparametric element formulation is used in this code. That is, the element calculations are carried out in terms of a local space coordinate, r, which has values of $-1, 0,$ and $+1$ at the left, center, and right-hand nodes, respectively.

The concentration interpolation functions are linear, and the displacement interpolation functions are quadratic. The resulting finite element is therefore *superparametric* in the concentration and *isoparametric* in displacement.

STATE VARIABLES, SVARS for dilatational strain are used in calculation of the ABAQUS "Jacobian" matrix AMATRX. State variables for stress, mass flux, and the gauss point locations are calculated for output purposes only. Some additional notes regarding the calculation of these state variables can be found near the end of the main body of the code.

```
C       DEGREES OF FREEDOM FOR MODEL IN ORDER:
C             (C1,U1,U2,C2,U3)



C
C       C       =       NODAL MASS FRACTION CONCENTRATION OF
C                               SOLUTE                  [kgSOLUTE/kgSOLID]
C       U       =       NODAL DISPLACEMENT                              [m]
C       KFLAG   =       CASE FLAG FOR PLANE STRESS OR PLANE STRAIN      [1]
C       AREA    =       CROSS-SECTIONAL AREA OF THE ROD                 [m^2]
C       E       =       YOUNG'S MODULUS FOR THE SOLID                   [Pa]
C       XNU     =       POISSON'S RATIO FOR THE SOLID                   [1]
C       D       =       DIFFUSION COEFFICIENT FOR SOLUTE IN SOLID [m^2/s]
C       ALPHA   =       SOLUTE EXPANSION COEFFICIENT                    [1]
C                       =(1/3)*(RHO*(PARTIAL MOLAR VOLUME OF SOLUTE))/XMW
C       CREF    =       REFERENCE CONCENTRATION         [kgSolid/kgSolute]
C       RHO     =       DENSITY OF SOLID MIXTURE                [kg/m^3]
C       XMW     =       MOLECULAR WEIGHT FOR SOLUTE SPECIES     [kg/mol]
C       TEMP    =       AMBIENT TEMPERATURE (ASSUMED CONSTANT)          [K]
C       TRAPS   =       TRAP SITES CONSTANT (CSRKR IN (1+CSRKR) TERM) [1]
C
      KFLAG  =int(PROPS(1))
      AREA   =PROPS(2)
      E      =PROPS(3)
      XNU    =PROPS(4)
      D      =PROPS(5)
      ALPHA  =PROPS(6)
      CREF   =PROPS(7)
      RHO    =PROPS(8)
      XMW    =PROPS(9)
      TEMP   =PROPS(10)
      TRAPS  =PROPS(11)


C       2-POINT GAUSSIAN INTEGRATION LOCATIONS AND WEIGHTS
C
     data GR/-0.577350269189626D0,0.577350269189626D0/,
     1     GW/ 1.000000000000000D0,1.000000000000000D0/



C
C       RS      =       GAS CONSTANT FOR SOLUTE SPECIES
C       BULK    =       BULK MODULUS FOR THE SOLID
C       XKON1   =       NON-DIMENSIONAL COEFFICIENT FOR (C*DE/DX) TERM OF
C                       MASS FLUX EQUATION
C                       (J=-DEFF*DC/DX + DEFF*XKON1*C*DE/DX)
C       DEFF    =       EFFECTIVE DIFFUSION COEFFICIENT
C
      RS     = 8.31432D0/XMW
      BULK   = E/(3.0D0*(1.0D0-2.0D0*XNU))
      XKON1  = 3.0D0*BULK*ALPHA/(RHO*RS*TEMP)
      DEFF   = D/(1.0D0+TRAPS )
```


The nodal dof are stored in the array `U(NDOF)` in the UEL subroutine:

$$\lfloor U(1), U(2), U(3), U(4), U(5) \rfloor = \lfloor c_1, u_1, u_2, c_2, u_3 \rfloor$$

This ordering is in agreement with standard ABAQUS and finite element conventions.

PROPERTIES for the element include material constants for the SOLID and pertinent SOLUTE data. These properties are specified in the "UEL PROPERTIES" option of the ABAQUS input deck and passed via the `PROPS(NPROPS)` array. Physical dimensions are specified here in SI units, but the program can be used with any dimensionally consistent system of units.

KFLAG represents the only non-physical "property" specified and indicates the desired linear elastic and coupling case to be run.

KFLAG values: 1 ⇒ Plane Stress, Fully Coupled
2 ⇒ Plane Strain, Fully Coupled
3 ⇒ Plane Stress, Weakly Coupled
4 ⇒ Plane Strain, Weakly Coupled
(Uncoupled analysis is achieved by setting `ALPHA=0` in the input deck)

GAUSS POINTS are standard two-point Gaussian locations and weights,

$$\texttt{GR(i)} = \pm\frac{1}{\sqrt{3}}, \quad \texttt{GW(i)} = 1.0$$

DEFINITIONS of calculated constants for the model.

$$\texttt{RS} = \frac{\mathbb{R}}{\texttt{XMW}}$$

$$\mathbb{R} \equiv \text{universal gas constant} = 8.31432\ [J/mol{\cdot}^{\circ}K]$$

BULK MODULUS is calculated using the elastic modulus and Poisson's ratio; it is used to simplify the coefficients (`B1, B2, B3`) in the constitutive equation for the stress.

DEFF is the effective diffusion coefficient defined by:

$$D_{eff} \equiv \frac{D}{(1 + c_R^* K_R)}$$

```
C
C       SET CONSTANTS FOR PLANE STRESS OR PLANE STRAIN CASE
C       1=> PLANE STRESS, FULLY COUPLED
C       2=> PLANE STRAIN, FULLY COUPLED
C       3=> PLANE STRESS, WEAKLY COUPLED
C       4=> PLANE STRAIN, WEAKLY COUPLED
C
      if(KFLAG.eq.1) then
            A1=(1.0D0-2.0D0*XNU)
            A2=(2.0D0*(1.0D0+XNU)*ALPHA)*(1.0D0+TRAPS)
            A3=(A2*CREF)
            B1=(3.0D0*BULK)
            B2=(9.0D0*BULK*ALPHA)*(1.0D0+TRAPS)
            B3=(B2*CREF)
      elseif(KFLAG.eq.2) then
            A1=1.0D0
            A2=0.0D0
            A3=0.0D0
            B1=(1.0D0-XNU)*E/((1.0D0+XNU)*(1.0D0-2.0D0*XNU))
            B2=(3.0D0*BULK*ALPHA)*(1.0D0+TRAPS)
            B3=(B2*CREF)
      elseif(KFLAG.eq.3) then
            A1=(1.0D0-2.0D0*XNU)
            A2= 0.0D0
            A3= 0.0D0
            B1=(3.0D0*BULK)
            B2= 0.0D0
            B3= 0.0D0
      elseif(KFLAG.eq.4) then
            A1=1.0D0
            A2=0.0D0
            A3=0.0D0
            B1=(1.0D0-XNU)*E/((1.0D0+XNU)*(1.0D0-2.0D0*XNU))
            B2= 0.0D0
            B3= 0.0D0
      endif


C
C       SET GLOBAL COORDINATES FOR NODES ON CURRENT ELEMENT
C
        X(1)=COORDS(1,1)+U(2)
        X(2)=COORDS(1,2)+U(3)
        X(3)=COORDS(1,3)+U(5)

C
C       SET GLOBAL COORDINATES FOR GAUSS POINTS ON CURRENT ELEMENT
C
        XGAUS(1)=H1(GR(1))*X(1)+H2(GR(1))*X(2)+H3(GR(1))*X(3)
        XGAUS(2)=H1(GR(2))*X(1)+H2(GR(2))*X(2)+H3(GR(2))*X(3)

C
C       CALCULATE INVERSE JACOBIAN AND DETERMINANT FOR ISOPARAMETRIC
C       TRANSFORMATION
C
         do 20 I = 1,2
              XJI(I)=1.0D0/XJACGR(I),X(1),X(2),X(3))
              DJ(I)=DETJ(GR(I),X(1),X(2),X(3))
   20     continue
```


CASE DETERMINATION is made possible by the fact that the hydrostatic strain and the stress for the 1-D case may be written using a set of defined coefficients.

$$e = A_1 \frac{\partial u}{\partial x} + A_2 c - A_3$$
$$\sigma = B_1 e - B_2 c + B_3$$

The values of A_i and B_i are assigned based on the value of KFLAG set in the input deck:

KFLAG = 1 $\Rightarrow$ Plane Stress, Fully Coupled
KFLAG = 2 $\Rightarrow$ Plane Strain, Fully Coupled
KFLAG = 3 $\Rightarrow$ Plane Stress, Weakly Coupled
KFLAG = 4 $\Rightarrow$ Plane Strain, Weakly Coupled
(Uncoupled analysis is achieved by setting ALPHA=0 in the input deck)

CALCULATION of NODAL COORDINATES is necessary for calculating the Jacobian of the coordinate transformation for the deformed configuration. ABAQUS passes in the COORDS(MCRD,NNODE) array which contains the original global coordinates of the nodes on the element. The displacement at each node must then be added to the original coordinate to give the nodal position in the deformed configuration.

CALCULATION of GAUSS POINT COORDINATES in terms of the global coordinate system is necessary for later calculations of the distributed load functions and for storage in the state variable array. This is performed using the quadratic interpolation functions.

JACOBIAN AND DETERMINANT OF TRANSFORMATION for the 1-D model are both scalar functions of the local element coordinate, r. The product of the inverse Jacobian and the determinant of the Jacobian is unity, and this product is directly simplified wherever it occurs in order to reduce the number of computations.

The inverse Jacobian will be denoted as $[J^{-1}]$, or $1/J(r_k)$ if Gauss integration is indicated, and the determinant will be denoted by $|J|$.

```
      if(LFLAGS(1).ne.71)then
C
CC      <<<<<<<<<<<  CALCULATE CAPACITANCE MATRIX >>>>>>>>>
C
      CAP(1,1)    = AREA*(G1(GR(1))*G1(GR(1))*DJ(1)*GW(1)
     1             + G1(GR(2))*G1(GR(2))*DJ(2)*GW(2))

      CAP(1,2)    = AREA*(G1(GR(1))*G2(GR(1))*DJ(1)*GW(1)
     1             + G1(GR(2))*G2(GR(2))*DJ(2)*GW(2))

      CAP(2,1)    = AREA*(G2(GR(1))*G1(GR(1))*DJ(1)*GW(1)
     1             + G2(GR(2))*G1(GR(2))*DJ(2)*GW(2))

      CAP(2,2)    = AREA*(G2(GR(1))*G2(GR(1))*DJ(1)*GW(1)
     1             + G2(GR(2))*G2(GR(2))*DJ(2)*GW(2))
      endif


C
C
CC      <<<<<<<<<<<  CALCULATE STIFFNESS MATRICES >>>>>>>>>
C
CC      CALCULATE de/dr USING VALUES FROM THE PREVIOUS TIME STEP
C
      E1=SVARS(1)
      E2=SVARS(2)
      DE = (E2-E1)/(GR(2)-GR(1))
```



```
C
CC      COEFFICIENTS OF CONCENTRATION D.O.F. IN MASS BALANCE EQUATION
C
      XKC(1,1)   = AREA*DEFF*(XJI(1)*(DG1(GR(1))*DG1(GR(1))
     1              -XKON1*DG1(GR(1))*DE*G1(GR(1)))*GW(1)
     2                +XJI(2)*(DG1(GR(2))*DG1(GR(2))
     3              -XKON1*DG1(GR(2))*DE*G1(GR(2)))*GW(2))

      XKC(1,2)   = AREA*DEFF*(XJI(1)*(DG1(GR(1))*DG2(GR(1))
     1              -XKON1*DG1(GR(1))*DE*G2(GR(1)))*GW(1)
     2                + XJI(2)*(DG1(GR(2))*DG2(GR(2))
     3              -XKON1*DG1(GR(2))*DE*G2(GR(2)))*GW(2))

      XKC(2,1)   = AREA*DEFF*(XJI(1)*(DG2(GR(1))*DG1(GR(1))
     1              -XKON1*DG2(GR(1))*DE*G1(GR(1)))*GW(1)
     2                + XJI(2)*(DG2(GR(2))*DG1(GR(2))
     3              -XKON1*DG2(GR(2))*DE*G1(GR(2)))*GW(2))

      XKC(2,2)   = AREA*DEFF*(XJI(1)*(DG2(GR(1))*DG2(GR(1))
     1              -XKON1*DG2(GR(1))*DE*G2(GR(1)))*GW(1)
     2                + XJI(2)*(DG2(GR(2))*DG2(GR(2))
     3              -XKON1*DG2(GR(2))*DE*G2(GR(2)))*GW(2))
```

CHECK `LFLAGS(1)` for ABAQUS analysis type. The numerical steps are minimized by skipping the calculation of the capacitance matrix if the indicated analysis is steady-state.

CAPACITANCE MATRIX contains the coefficients of the $\partial c/\partial t$ term in the mass balance equation. Each term of the 2×2 matrix is calculated by numerical integration.

$$[C_c] \equiv A_e \int_{-1}^{+1} \{g_i(r)\}\lfloor g_i(r)\rfloor |\, J\,| dr \equiv \sum_{k=1}^{2} A_e W_k \Big(\{g_i(r_k)\}\lfloor g_i(r_k)\rfloor J(r_k) \Big)$$

END `LFLAGS(1)` CAPACITANCE MATRIX SKIP

STIFFNESS MATRIX $[K]$ must be calculated for both transient and steady-state analyses.

The dilatational strain gradient $\partial e/\partial r$ is assumed constant across the length of an element and is approximated using the first order difference, $\Delta e/\Delta r$, using values of e from the previous time step. The local gradient, $\Delta e/\Delta r$, is calculated and then transformed to $\Delta e/\Delta x$ in the following calculations via multiplication by the inverse Jacobian.

Stiffness Matrix $[K_{cu}]$ Calculations: Displacement coupling in the mass balance equation occurs through the $\partial e/\partial x$ term. The approximation of $\partial e/\partial x$, as described above, eliminates any $[K_{cu}]$ contribution to the total stiffness matrix $[K]$. That is, $[K_{cu}] = [0]$.

Stiffness Matrix $[K_c]$ Calculations: contributions from the concentration dof in the mass balance equation. Numerical integration is performed using a two-point Gaussian scheme:

$$[K_c] \equiv A_e \int_{-1}^{+1} [\,J^{-1}]^2 D_{eff} \left(\left\{ \frac{dg_i(r)}{dr} \right\} \left\lfloor \frac{dg_i(r)}{dr} \right\rfloor - K_1 \left\{ \frac{dg_i(r)}{dr} \right\} \frac{\partial e}{\partial r} \lfloor g_i(r) \rfloor \right) |\, J\,| dr$$

$$[K_c] = \sum_{k=1}^{2} A_e W_k \left(D_{eff} \left(\left\{ \frac{dg_i(r_k)}{dr} \right\} \left\lfloor \frac{dg_i(r_k)}{dr} \right\rfloor - K_1 \left\{ \frac{dg_i(r_k)}{dr} \right\} \frac{\partial e}{\partial r} \lfloor g_i(r_k) \rfloor \right) \frac{1}{J(r_k)} \right)$$

```
C
C
C       COEFFICIENTS OF CONCENTRATION IN LINEAR ELASTIC EQUATION
C
C

      XKUC(1,1) = AREA*(B1*A2-B2)*((DH1(GR(1))*G1(GR(1)))*GW(1)
     1                    + (DH1(GR(2))*G1(GR(2)))*GW(2))

      XKUC(1,2) = AREA*(B1*A2-B2)*((DH1(GR(1))*G2(GR(1)))*GW(1)
     1                    + (DH1(GR(2))*G2(GR(2)))*GW(2))

      XKUC(2,1) = AREA*(B1*A2-B2)*((DH2(GR(1))*G1(GR(1)))*GW(1)
     1                    + (DH2(GR(2))*G1(GR(2)))*GW(2))

      XKUC(2,2) = AREA*(B1*A2-B2)*((DH2(GR(1))*G2(GR(1)))*GW(1)
     1                    + (DH2(GR(2))*G2(GR(2)))*GW(2))

      XKUC(3,1) = AREA*(B1*A2-B2)*((DH3(GR(1))*G1(GR(1)))*GW(1)
     1                    + (DH3(GR(2))*G1(GR(2)))*GW(2))

      XKUC(3,2) = AREA*(B1*A2-B2)*((DH3(GR(1))*G2(GR(1)))*GW(1)
     1                    + (DH3(GR(2))*G2(GR(2)))*GW(2))


C
C       COEFFICIENTS OF DISPLACEMENT IN LINEAR ELASTIC EQUATION
C

      XKU(1,1)  = AREA*B1*A1*(XJI(1)*(DH1(GR(1))*DH1(GR(1)))*GW(1)
     1                + XJI(2)*(DH1(GR(2))*DH1(GR(2)))*GW(2))

      XKU(1,2)  = AREA*B1*A1*(XJI(1)*(DH1(GR(1))*DH2(GR(1)))*GW(1)
     1                + XJI(2)*(DH1(GR(2))*DH2(GR(2)))*GW(2))

      XKU(1,3)  = AREA*B1*A1*(XJI(1)*(DH1(GR(1))*DH3(GR(1)))*GW(1)
     1                + XJI(2)*(DH1(GR(2))*DH3(GR(2)))*GW(2))

      XKU(2,1)  = AREA*B1*A1*(XJI(1)*(DH2(GR(1))*DH1(GR(1)))*GW(1)
     1                + XJI(2)*(DH2(GR(2))*DH1(GR(2)))*GW(2))

      XKU(2,2)  = AREA*B1*A1*(XJI(1)*(DH2(GR(1))*DH2(GR(1)))*GW(1)
     1                + XJI(2)*(DH2(GR(2))*DH2(GR(2)))*GW(2))

      XKU(2,3)  = AREA*B1*A1*(XJI(1)*(DH2(GR(1))*DH3(GR(1)))*GW(1)
     1                + XJI(2)*(DH2(GR(2))*DH3(GR(2)))*GW(2))

      XKU(3,1)  = AREA*B1*A1*(XJI(1)*(DH3(GR(1))*DH1(GR(1)))*GW(1)
     1                + XJI(2)*(DH3(GR(2))*DH1(GR(2)))*GW(2))

      XKU(3,2)  = AREA*B1*A1*(XJI(1)*(DH3(GR(1))*DH2(GR(1)))*GW(1)
     1                + XJI(2)*(DH3(GR(2))*DH2(GR(2)))*GW(2))

      XKU(3,3)  = AREA*B1*A1*(XJI(1)*(DH3(GR(1))*DH3(GR(1)))*GW(1)
     1                + XJI(2)*(DH3(GR(2))*DH3(GR(2)))*GW(2))
C
```

Stiffness Matrix $[K_{uc}]$ Calculations: contributions from the concentration dof in the linear momentum balance equation. Numerical integration is performed using a two-point Gaussian scheme:

$$[K_{uc}] \equiv A_e \int_{-1}^{+1} (B_1 A_2 - B_2)[J^{-1}] \left\{ \frac{dh_j(r)}{dr} \right\} \lfloor g_i(r) \rfloor \mid J \mid dr$$

$$[K_{uc}] = \sum_{k=1}^{2} A_e W_k \left((B_1 A_2 - B_2) \left\{ \frac{dh_j(r_k)}{dr} \right\} \lfloor g_i(r_k) \rfloor \right)$$

Stiffness Matrix $[K_u]$ Calculations: contributions from the displacement dof in the linear momentum balance equation. Numerical integration is performed using a two-point Gaussian scheme:

$$[K_u] \equiv A_e \int_{-1}^{+1} (B_1 A_1)[J^{-1}]^2 \left\{ \frac{dh_j(r)}{dr} \right\} \left\lfloor \frac{dh_j(r)}{dr} \right\rfloor \mid J \mid dr$$

$$[K_u] = \sum_{k=1}^{2} A_e W_k \left((B_1 A_1) \left\{ \frac{dh_j(r_k)}{dr} \right\} \left\lfloor \frac{dh_j(r_k)}{dr} \right\rfloor \frac{1}{J(r_k)} \right)$$

```
C
      if(LFLAGS(1).eq.71) then


C                 ********************************
C                 ********************************
C      ************** STEADY STATE DIFFUSION ********************
C                 ********************************
C
      if (LFLAGS(3).eq.1.or.LFLAGS(3).eq.2) then
C
C       <<<<<< CALCULATE AMATRX = [K] >>>>>>>>>>>>
C       WHERE [K] IS
C             [XKC(1,1)  0       0       XKC(1,2)  0       ]
C             [XKUC(1,1) XKU(1,1) XKU(1,2) XKUC(1,2) XKU(1,3)]
C             [XKUC(2,1) XKU(2,1) XKU(2,2) XKUC(2,2) XKU(2,3)]
C             [XKC(2,1)  0       0       XKC(2,2)  0       ]
C             [XKUC(3,1) XKU(3,1) XKU(3,2) XKUC(3,2) XKU(3,3)]

      AMATRX(1,1) = XKC(1,1)
      AMATRX(1,4) = XKC(1,2)
      AMATRX(2,1) = XKUC(1,1)
      AMATRX(2,2) = XKU(1,1)
      AMATRX(2,3) = XKU(1,2)
      AMATRX(2,4) = XKUC(1,2)
      AMATRX(2,5) = XKU(1,3)
      AMATRX(3,1) = XKUC(2,1)
      AMATRX(3,2) = XKU(2,1)
      AMATRX(3,3) = XKU(2,2)
      AMATRX(3,4) = XKUC(2,2)
      AMATRX(3,5) = XKU(2,3)
      AMATRX(4,1) = XKC(2,1)
      AMATRX(4,4) = XKC(2,2)
      AMATRX(5,1) = XKUC(3,1)
      AMATRX(5,2) = XKU(3,1)
      AMATRX(5,3) = XKU(3,2)
      AMATRX(5,4) = XKUC(3,2)
      AMATRX(5,5) = XKU(3,3)


      endif

C
      if((LFLAGS(3).eq.1).or.(LFLAGS(3).eq.5)) then
C
```

CHECK `LFLAGS(1)` for ABAQUS analysis type. If the analysis type is steady-state coupled deformation/ heat transfer, then assign the steady state matrices.

STEADY STATE MATRIX ASSIGNMENTS

CHECK `LFLAGS(3)` for ABAQUS information request. If needed, assign AMATRX for return to main program.

`AMATRX` ASSIGNMENT for steady state analysis is a direct assignment of the previously calculated stiffness matrix components:

$$\text{AMATRX} = \begin{bmatrix} K_c^{11} & 0 & 0 & K_c^{12} & 0 \\ K_{uc}^{11} & K_u^{11} & K_u^{12} & K_{uc}^{12} & K_u^{13} \\ K_{uc}^{21} & K_u^{21} & K_u^{22} & K_{uc}^{22} & K_u^{23} \\ K_c^{21} & 0 & 0 & K_c^{22} & 0 \\ K_{uc}^{31} & K_u^{31} & K_u^{32} & K_{uc}^{32} & K_u^{33} \end{bmatrix}$$

where, for example, K_c^{21} represents the term in the second row, first column of the K_c matrix.

END `LFLAGS(3)` `AMATRX` ASSIGNMENT

CHECK `LFLAGS(3)` for ABAQUS information request. If needed, assign RHS array for return to main program.

```
C
C            <<<<<< CALCULATE {RHS} = {R}-[K]{U} >>>>>>>>>>>>
C
C     NOTE: THIS USER ELEMENT SUBROUTINE ASSUMES THAT ALL OF
C           NEUMANN BOUNDARY DATA ARE HOMOGENEOUS (i.e., ZERO).
C           INHOMOGENEOUS (NON-ZERO) NEUMANN BOUNDARY DATA SUCH
C           AS NON-ZERO BOUNDARY TRACTIONS AND/OR SOLUTE FLUXES
C           ARE AUTOMATICALLY INCORPORATED INTO THE COMPUTATIONS
C           BY ABAQUS. INHOMOGENEOUS DATA SHOULD BE ENTERED IN
C           THE INPUT DECK AS CONCENTRATED NODAL FORCES.
C
C      THE FOLLOWING SECTION CALCULATES THE TOTAL USER SUPPLIED
C      DISTRIBUTED LOADS (e.g. BODY FORCES) AT THE GAUSS POINTS
C      ON THE ROD FOR USE IN FINDING THE RHS VECTOR.
C

      FUN=0.0D0
       do 31 I=1,2
          F(I) = 0.0D0
          FNU(I) = 0.0D0
   31  continue

       do 41 K1=1,MDLOAD
            if(JDLTYP(K1,1).gt.0)then
                FUN=FUN+ADLMAG(K1,1)
            elseif(JDLTYP(K1,1).lt.0)then
                call KFCALC(JDLTYP(K1,1),F,XGAUS,TIME(2))
                do 51 I=1,2
                   FNU(I)=FNU(I)+F(I)
   51           continue
            endif
   41    continue



       do 61 I=1,2
          FNU(I)=FNU(I)+FUN
   61    continue
```


CALCULATION OF THE RIGHT-HAND SIDE (RHS) VECTOR

DISTRIBUTED LOADS must be converted to consistent nodal loads for use in calculation of the $\{R_u\}$ matrix. ABAQUS recognizes two types of distributed loads:

1. those with constant magnitude across the element. The magnitude is specified in the array ADLMAG and the variable JDLTYP > 0;
2. those with magnitude specified in the UEL subroutine as a function of the global coordinate, x, and time, t. The variable JDLTYP < 0.

ZERO THE ARRAYS which will contain the values of the total loads at the Gauss points.

COMBINED TOTAL OF JDLTYP > 0 AND JDLTYP < 0 DISTRIBUTED LOADS: is given by the integer variable, MDLOAD.

TYPE JDLTYP > 0 DISTRIBUTED LOADS: The total magnitude of type JDLTYP > 0 loads is found by summation.

TYPE JDLTYP < 0 DISTRIBUTED LOADS: The total magnitude of type JDLTYP < 0 loads is found by summing magnitudes at each Gauss point location. The subroutine KFCALC is called to determine the value of the load at each Gauss point. See the notes for subroutine KFCALC for additional explanation.

TOTAL DISTRIBUTED LOAD at each Gauss point is determined by adding the total JDLTYP > 0 loads to the total JDLTYP < 0 types loads. This is the load value that needs to be used in the calculations of $\{R_u\}$.

CONSISTENT NODAL LOADS are calculated by integrating the product of the nodal interpolation function and the distributed load over the element. The total distributed load *at each Gauss point* is required for the Gaussian integration.

```
C
      R(1) = 0.0D0
C
      R(2)= AREA*((H1(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH1(GR(1)))*DJ(1)*GW(1)
     2       +(H1(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH1(GR(2)))*DJ(2)*GW(2))
C
      R(3)= AREA*((H2(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH2(GR(1)))*DJ(1)*GW(1)
     2       +(H2(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH2(GR(2)))*DJ(2)*GW(2))
C
      R(4) = 0.0D0
C
      R(5)= AREA*((H3(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH3(GR(1)))*DJ(1)*GW(1)
     2       +(H3(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH3(GR(2)))*DJ(2)*GW(2))
C
C
      RHS(1,1) = R(1) -XKC(1,1)*U(1)-XKC(1,2)*U(4)
C
      RHS(2,1) = R(2) -XKUC(1,1)*U(1)-XKU(1,1)*U(2)-XKU(1,2)*U(3)
     1                -XKUC(1,2)*U(4)-XKU(1,3)*U(5)
C
      RHS(3,1) = R(3) -XKUC(2,1)*U(1)-XKU(2,1)*U(2)-XKU(2,2)*U(3)
     1                -XKUC(2,2)*U(4)-XKU(2,3)*U(5)
C
      RHS(4,1) = R(4) -XKC(2,1)*U(1)-XKC(2,2)*U(4)
C
      RHS(5,1) = R(5) -XKUC(3,1)*U(1)-XKU(3,1)*U(2)-XKU(3,2)*U(3)
     1                -XKUC(3,2)*U(4)-XKU(3,3)*U(5)
C
C
      endif
```

CALCULATION of $\{\mathcal{R}\}$: The array R(NDOF) is determined using the column matrices $\{R_c\}$ and $\{R_u\}$ through the equation:

$$\mathrm{R}(i)=\lfloor\, R_c^1 \quad R_u^1 \quad R_u^2 \quad R_c^2 \quad R_u^3 \,\rfloor^{\dagger}$$

where:

$$\{R_c\} \equiv -A_e\,\mathcal{J}_L^*\,\{g_i(r)\}\Big|_{-1}^{+1}$$

$$\{R_u\} \equiv A_e \int_{-1}^{+1} \left(\{h_j(r)\}F_x - (B_3 - B_1 A_3)[\,J^{-1}]\left\{\frac{dh_j(r)}{dr}\right\}\right) |\,J\,|\,dr + A_e\,\sigma_x\,\{h_j(r)\}\Big|_{-1}^{+1}$$

The code does not incorporate the inhomogeneous Neumann boundary data included in the $\{R_c\}$ and $\{R_u\}$ expressions into the code. These are added directly by ABAQUS using the concentrated nodal load data specified in the input deck under the CLOAD option. As a result:

$$\{R_c\} = \{0\}$$

$$\{R_u\} = \sum_{k=1}^{2} W_k \left(\{h_j(r_k)\}F_x - \frac{B_3 - B_1 A_3}{J(r_k)}\left\{\frac{dh_j(r_k)}{dr}\right\}\right) A_e\,|J(r_k)|$$

The quantity $A_e\,\mathcal{J}_L^*\Big|_{-1}^{+1}$ is proportional to the net solute flow out of the element. Actual mass flow rates are given by $\rho\,(1 + c_R^s K_R)\,\mathcal{J}_L^*$ in $[mass\,Solute/(area \times time)]$ units.

The quantity $A_e\,\sigma_x$ represents a boundary force.

CALCULATION OF RHS (NDOF) ARRAY *requires matrix multiplication, since*

$$\{\mathrm{RHS}\}=\{\mathcal{R}\} - [\mathcal{K}]\{\mathrm{U}\}$$

where U(NDOF) is the vector of nodal concentrations and displacements from the previous iteration, and $[\mathcal{K}]$ is the element stiffness matrix (same form as AMATRX above).

END LFLAGS(3) RHS ASSIGNMENT

END LFLAGS(1) STEADY STATE MATRIX ASSIGNMENTS

```
      elseif((LFLAGS(1).eq.72).or.(LFLAGS(1).eq.73)) then


C
C           ********************************
C     ************* TRANSIENT DIFFUSION ********************
C           ********************************
C


      if (LFLAGS(3).eq.1.or.LFLAGS(3).eq.2) then


C
C        <<<<<< CALCULATE AMATRX = [[K]+[C]/DTIME] >>>>>>>>>>>>
C        WHERE [K] IS
C              [XKC(1,1)  0        0        XKC(1,2)  0       ]
C              [XKUC(1,1) XKU(1,1) XKU(1,2) XKUC(1,2) XKU(1,3)]
C              [XKUC(2,1) XKU(2,1) XKU(2,2) XKUC(2,2) XKU(2,3)]
C              [XKC(2,1)  0        0        XKC(2,2)  0       ]
C              [XKUC(3,1) XKU(3,1) XKU(3,2) XKUC(3,2) XKU(3,3)]
C
C
C
C        AND [C] IS
C              [CAP(1,1) 0        0        CAP(1,2) 0]
C              [0        0        0        0        0]
C              [0        0        0        0        0]
C              [CAP(2,1) 0        0        CAP(2,2) 0]
C              [0        0        0        0        0]
C
C
C
C
      AMATRX(1,1) = XKC(1,1) + CAP(1,1)/DTIME
      AMATRX(1,4) = XKC(1,2) + CAP(1,2)/DTIME
      AMATRX(2,1) = XKUC(1,1)
      AMATRX(2,2) = XKU(1,1)
      AMATRX(2,3) = XKU(1,2)
      AMATRX(2,4) = XKUC(1,2)
      AMATRX(2,5) = XKU(1,3)
      AMATRX(3,1) = XKUC(2,1)
      AMATRX(3,2) = XKU(2,1)
      AMATRX(3,3) = XKU(2,2)
      AMATRX(3,4) = XKUC(2,2)
      AMATRX(3,5) = XKU(2,3)
      AMATRX(4,1) = XKC(2,1) + CAP(2,1)/DTIME
      AMATRX(4,4) = XKC(2,2) + CAP(2,2)/DTIME
      AMATRX(5,1) = XKUC(3,1)
      AMATRX(5,2) = XKU(3,1)
      AMATRX(5,3) = XKU(3,2)
      AMATRX(5,4) = XKUC(3,2)
      AMATRX(5,5) = XKU(3,3)

      endif
C
C
```


CHECK LFLAGS(1) for ABAQUS analysis type. If the analysis type is transient coupled deformation/heat transfer, then assign the TRANSIENT matrices.

TRANSIENT MATRIX ASSIGNMENTS

CHECK LFLAGS(3) for ABAQUS information request. If needed, assign AMATRX for return to main program.

AMATRX ASSIGNMENT for transient analysis requires combining the previously calculated stiffness and capacitance matrix components such that:

$$\text{AMATRX} = \begin{bmatrix} K_c^{11}+\frac{1}{\Delta t}C_c^{11} & 0 & 0 & K_c^{12}+\frac{1}{\Delta t}C_c^{12} & 0 \\ K_{uc}^{11} & K_u^{11} & K_u^{12} & K_{uc}^{12} & K_u^{13} \\ K_{uc}^{21} & K_u^{21} & K_u^{22} & K_{uc}^{22} & K_u^{23} \\ K_c^{21}+\frac{1}{\Delta t}C_c^{21} & 0 & 0 & K_c^{22}+\frac{1}{\Delta t}C_c^{22} & 0 \\ K_{uc}^{31} & K_u^{31} & K_u^{32} & K_{uc}^{32} & K_u^{33} \end{bmatrix}$$

where, for example, K_c^{21} represents the term in the second row, first column of the K_c matrix. The presence of capacitance terms distinguish this array from the steady state version of AMATRX.

END LFLAGS(3) AMATRX ASSIGNMENT

```
C
      if((LFLAGS(3).eq.1).or.(LFLAGS(3).eq.5)) then
C
C
C       <<<<<< CALCULATE {RHS} = {R}-[K]{U}-([C]/DTIME){DU}>>>>>>
C
C      THE FOLLOWING SECTION CALCULATES THE  TOTAL USER SUPPLIED
C      DISTRIBUTED LOADS (e.g. BODY FORCES) AT THE GAUSS POINTS
C      ON THE ROD FOR USE IN FINDING THE RHS VECTOR.
C
C
      FUN=0.0D0
       do 131 I=1,2
          F(I) = 0.0D0
          FNU(I) = 0.0D0
 131   continue
C
       do 141 K1=1,MDLOAD
            if(JDLTYP(K1,1).gt.0)then
                FUN=FUN+ADLMAG(K1,1)
            elseif(JDLTYP(K1,1).lt.0)then
                call KFCALC(JDLTYP(K1,1),F,XGAUS,TIME(2))
                do 151 I=1,2
                   FNU(I)=FNU(I)+F(I)
 151            continue
            endif
 141    continue
C
C
       do 161 I=1,2
          FNU(I)=FNU(I)+FUN
 161    continue
C
```


CHECK `LFLAGS(3)` for ABAQUS information request. If needed, assign `RHS` values.

CALCULATION OF THE RIGHT-HAND SIDE (RHS) VECTOR

DISTRIBUTED LOADS must be converted to consistent nodal loads for use in calculation of the $\{R_u\}$ matrix. ABAQUS recognizes two types of distributed loads:

1. those with constant magnitude across the element. The magnitude is specified in the array `ADLMAG` and the variable `JDLTYP` > 0;
2. those with magnitude specified in the `UEL` subroutine as a function of the global coordinate, x, and time, t. The variable `JDLTYP` < 0.

ZERO THE ARRAYS which will contain the values of the total loads at the Gauss points.

COMBINED TOTAL OF `JDLTYP` > 0 AND `JDLTYP` < 0 DISTRIBUTED LOADS: is given by the integer variable, `MDLOAD`.

TYPE `JDLTYP` > 0 DISTRIBUTED LOADS: The total magnitude of type `JDLTYP` > 0 loads is found by summation.

TYPE `JDLTYP` < 0 DISTRIBUTED LOADS: The total magnitude of type `JDLTYP` < 0 loads is found by summing magnitudes at each Gauss point location. The `subroutine KFCALC` is called to determine the value of the load at each Gauss point. See the notes for `subroutine KFCALC` for additional explanation.

TOTAL DISTRIBUTED LOAD at each Gauss point is determined by adding the total `JDLTYP` > 0 loads to the total `JDLTYP` < 0 types loads. This is the load value that needs to be used in the calculations of $\{R_u\}$.

CONSISTENT NODAL LOADS are calculated by integrating the product of the nodal interpolation function and the distributed load over the element. The total distributed load *at each Gauss point* is required for the Gaussian integration.

```
C
      R(1) = 0.0D0
C
      R(2)= AREA*((H1(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH1(GR(1)))*DJ(1)*GW(1)
     2       +(H1(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH1(GR(2)))*DJ(2)*GW(2))
C
      R(3)= AREA*((H2(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH2(GR(1)))*DJ(1)*GW(1)
     2       +(H2(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH2(GR(2)))*DJ(2)*GW(2))
C
      R(4) = 0.0D0
C
      R(5)= AREA*((H3(GR(1))*FNU(1)
     1       -(B3-B1*A3)*XJI(1)*DH3(GR(1)))*DJ(1)*GW(1)
     2       +(H3(GR(2))*FNU(2)
     3       -(B3-B1*A3)*XJI(2)*DH3(GR(2)))*DJ(2)*GW(2))
C
C
      RHS(1,1) = R(1) -XKC(1,1)*U(1)-XKC(1,2)*U(4)
     1                -1.0D0/DTIME*(CAP(1,1)*DU(1,1)+CAP(1,2)*DU(4,1))
C
      RHS(2,1) = R(2) -XKUC(1,1)*U(1)-XKU(1,1)*U(2)-XKU(1,2)*U(3)
     1                -XKUC(1,2)*U(4)-XKU(1,3)*U(5)
C
      RHS(3,1) = R(3) -XKUC(2,1)*U(1)-XKU(2,1)*U(2)-XKU(2,2)*U(3)
     1                -XKUC(2,2)*U(4)-XKU(2,3)*U(5)
C
      RHS(4,1) = R(4) -XKC(2,1)*U(1)-XKC(2,2)*U(4)
     1                -1.0D0/DTIME*(CAP(2,1)*DU(1,1)+CAP(2,2)*DU(4,1))
C
      RHS(5,1) = R(5) -XKUC(3,1)*U(1)-XKU(3,1)*U(2)-XKU(3,2)*U(3)
     1                -XKUC(3,2)*U(4)-XKU(3,3)*U(5)
C
C
      endif
C
C     <<<<<< CHECK THAT PROCEDURE FLAG SENT MATCHES PROCEDURE PERFORMED >>>
C
      elseif((LFLAGS(1).ne.71).and.
     1    (LFLAGS(1).ne.72).and.(LFLAGS(1).ne.73)) then
      write(*,*) 'ERROR IN THE VALUE OF LFLAGS(1) = ',LFLAGS(1)
        endif
```

CALCULATION of $\{\mathcal{R}\}$: The array R(NDOF) is determined using the column matrices $\{R_c\}$ and $\{R_u\}$ through the equation:

$$\mathrm{R}(i)=\lfloor\, R_c^1 \quad R_u^1 \quad R_u^2 \quad R_c^2 \quad R_u^3 \,\rfloor^{\dagger}$$

where:

$$\{R_c\} \equiv -A_e\,\mathcal{J}_L^*\,\{g_i(r)\}\Big|_{-1}^{+1}$$

$$\{R_u\} \equiv A_e \int_{-1}^{+1} \left(\{h_j(r)\}F_x - (B_3 - B_1A_3)[J^{-1}]\left\{\frac{dh_j(r)}{dr}\right\}\right) |J|\,dr + A_e\,\sigma_x\,\{h_j(r)\}\Big|_{-1}^{+1}$$

The code does not incorporate the inhomogeneous Neumann boundary data included in the $\{R_c\}$ and $\{R_u\}$ expressions into the code. These are added directly by ABAQUS using the concentrated nodal load data specified in the input deck under the CLOAD option. As a result:

$$\{R_c\} = \{0\}$$

$$\{R_u\} = \sum_{k=1}^{2} W_k \left(\{h_j(r_k)\}F_x - \frac{B_3 - B_1A_3}{J(r_k)}\left\{\frac{dh_j(r_k)}{dr}\right\}\right) A_e\,|J(r_k)|$$

The quantity $A_e\,\mathcal{J}_L^*\Big|_{-1}^{+1}$ is proportional to the net solute flow out of the element. Actual mass flow rates are given by $\rho\,(1 + c_R^s K_R)\,\mathcal{J}_L^*$ in $[mass\,Solute/(area \times time)]$ units.

The quantity $A_e\,\sigma_x$ represents a boundary force.

CALCULATION OF RHS (NDOF) ARRAY requires matrix multiplication, since

$$\{\mathrm{RHS}\}=\{\mathcal{R}\} - [\mathcal{K}]\{\mathrm{U}\} - \frac{1}{\Delta t}[\mathcal{C}]\{\Delta \mathrm{U}\}$$

where U(NDOF) is the vector of nodal concentrations and displacements from the previous iteration, $[\mathcal{K}]$ is the element stiffness matrix, and $[\mathcal{C}]$ is the element capacitance matrix. $\{\Delta \mathrm{U}\}$ represents the ABAQUS array DU which is defined as the *change* in the nodal values from the previous increment.

END LFLAGS(3) RHS ASSIGNMENT

END LFLAGS(1) TRANSIENT MATRIX ASSIGNMENTS

CHECK LFLAGS(1) for ABAQUS analysis type. If the analysis type is neither steady-state nor transient coupled deformation/heat transfer, then set-off an error message indicating that this user element subroutine is incapable of performing the requested analysis.

```
C
      if(LFLAGS(3).eq.1) then

C
C     <<<<<<<<<<<  CALCULATE THE STATE VARIABLES >>>>>>>>>>>
C
C        DILATATIONAL STRAINS:
         SVARS(1) =  A1*XJI(1)*(DH1(GR(1))*U(2)
     1                    +DH2(GR(1))*U(3)+DH3(GR(1))*U(5))
     2              +A2*(G1(GR(1))*U(1)+G2(GR(1))*U(4))-A3
         SVARS(2) =  A1*XJI(2)*(DH1(GR(2))*U(2)+
     1                    DH2(GR(2))*U(3)+DH3(GR(2))*U(5))
     2              +A2*(G1(GR(2))*U(1)+G2(GR(2))*U(4))-A3

C        GAUSS POINT STRESSES:
         SVARS(3) = B1*SVARS(1)-B2*(G1(GR(1))*U(1)+G2(GR(1))*U(4))+B3
         SVARS(4) = B1*SVARS(2)-B2*(G1(GR(2))*U(1)+G2(GR(2))*U(4))+B3

C        OUTER NODE STRESSES:
         DE = (SVARS(2)-SVARS(1))/(GR(2)-GR(1))
         SVARS(5) = B1*(SVARS(1)+(-1.0D0-GR(1))*DE)-B2*U(1)+B3
         SVARS(6) = B1*(SVARS(2)+( 1.0D0-GR(2))*DE)-B2*U(4)+B3

C        CENTROIDAL SOLUTE MASS FLUX:
         SVARS(7)=D*(1.0D0/XJAC0.0D0,X(1),X(2),X(3)))
     1           *(-(DG1(0.0D0)*U(1)+DG2(0.0D0)*U(4))+
     2             XKON1*(G1(0.0D0)*U(1)+G2(0.0D0)*U(4))*DE)

C       GLOBAL GAUSS POINT LOCATIONS
        SVARS(8)= XGAUS(1)
        SVARS(9)= XGAUS(2)

C
C
      endif
      return
      end
C
C
C       ************************************************
```

CHECK LFLAGS(3) for ABAQUS information request. Update the state variables.

DILATATIONAL STRAIN is the only state variable actually used in the finite element calculations. All other state variables are calculated for output purposes only. Dilatational strain is calculated at the Gauss points for accuracy, using the equation:

$$e = A_1 \left\lfloor \frac{dH_j(x)}{dx} \right\rfloor \{u_j(t)\} + A_2 \lfloor G_i(x) \rfloor \{c_i(t)\} - A_3$$

AXIAL STRESS is calculated at the Gauss points for accuracy, using the equation:

$$\sigma_x = B_1 e - B_2 \lfloor G_i(x) \rfloor \{c_i(t)\} + B_3$$

AXIAL STRESS at the LHS element boundary node is calculated by replacing e in the above equation with the value:

$$e(r = -1) = e(r_1) - \left(\frac{\Delta e}{\Delta r}\right)(r_1 + 1)$$

and then evaluating $\lfloor G_i(x) \rfloor$ at the element boundary. A similar calculation scheme is used for the RHS nodal stress.

SOLUTE MASS FLUX is calculated at the center of the element from the equation:

$$\mathcal{J}_L = -D \left\lfloor \frac{dG_i(x)}{dx} \right\rfloor \{c_i(t)\} + D\, K_1 \lfloor G_i(x) \rfloor \{c_i(t)\} \frac{\partial e}{\partial x}$$

GAUSS POINT LOCATIONS are calculated and printed with the Gauss point state variable data. This calculation is performed at the beginning of `subroutine UEL` using a quadratic shape function approximation in the axial coordinate, x.

END OF THE MAIN PART OF SUBROUTINE UEL

```
C
      double precision function XJAC(R,X1,X2,X3)
      double precision R,X1,X2,X3
C     CALCULATE JACOBIAN OF ISOPARAMETRIC TRANSFORMATION
C          (D/DR=JAC^(-1)*D/DX)
            XJAC=(R-1.0D0/2.0D0)*X1-2.0D0*R*X2+(R+1.0D0/2.0D0)*X3
      return
      end
C
C
```

ISOPARAMETRIC TRANSFORM JACOBIAN between the global coordinate, x, and the local coordinate, r is given by:

$$[J] \equiv \left[\frac{dx}{dr}\right] = \left[\frac{dh_j(r)}{dr}\right]\{x_j(t)\}$$

In the present situation, the Jacobian is a scalar function of the local coordinate, r, equal to:

$$J = \left(r - \frac{1}{2}\right)x_1 - (2r)x_2 + \left(r + \frac{1}{2}\right)x_3$$

$$[J^{-1}] = \frac{1}{J}$$

```
C
C
      double precision function DETJ(R,X1,X2,X3)
      double precision R,X1,X2,X3
C     CALCULATE DETERMINANT OF JACOBIAN OF ISOPARAMETRIC TRANSFORMATION
C     (DR=DETJ*DX)
           DETJ=(R-1.0D0/2.0D0)*X1-2.0D0*R*X2+(R+1.0D0/2.0D0)*X3
      return
      end
C
C
```

DETERMINANT of the JACOBIAN is a scalar function of the local coordinate, r, and is equal to J:

$$|J| = J$$


```
C
C     LINEAR INTERPOLATION FUNCTIONS FOR CONCENTRATION
C
      double precision function G1(R)
      double precision R
            G1=(1.0D0/2.0D0)*(1.0D0-R)
      return
      end
C
C
      double precision function G2(R)
      double precision R
            G2=(1.0D0/2.0D0)*(1.0D0+R)
      return
      end
C
C
```

LINEAR *SUPERPARAMETRIC* INTERPOLATION FUNCTIONS are defined for the concentration:

$$g_1(r) \equiv \frac{1}{2}(1-r)$$

$$g_2(r) \equiv \frac{1}{2}(1+r)$$

```
C      QUADRATIC INTERPOLATION FUNCTIONS FOR DISPLACEMENT
C
      double precision function H1(R)
      double precision R
            H1=1.0D0/2.0D0*(R**2-R)
      return
      end
C
      double precision function H2(R)
      double precision R
             H2=1.0D0-R**2
      return
      end
C
      double precision function H3(R)
      double precision R
            H3=1.0D0/2.0D0*(R**2+R)
      return
      end


C
C     DERIVATIVES OF LINEAR INTERPOLATIONS FOR CONCENTRATION
C
      double precision function DG1(R)
      double precision R
            DG1=(-1.0D0/2.0D0)
      return
      end
C
      double precision function DG2(R)
      double precision R
            DG2=(1.0D0/2.0D0)
      return
      end


C
C     DERIVATIVES OF QUADRATIC INTERPOLATIONS FOR DISPLACEMENT
C
      double precision function DH1(R)
      double precision R
            DH1=(R-1.0D0/2.0D0)
      return
      end
C
      double precision function DH2(R)
      double precision R
            DH2=-2.0D0*R
      return
      end
C
      double precision function DH3(R)
      double precision R
            DH3=(R+1.0D0/2.0D0)
      return
      end
```


QUADRATIC *ISOPARAMETRIC* INTERPOLATION FUNCTIONS are defined for the displacement:

$$h_1(r) \equiv \frac{1}{2}(r^2 - r)$$
$$h_2(r) \equiv (1 - r^2)$$
$$h_3(r) \equiv \frac{1}{2}(r^2 + r)$$

INTERPOLATION FUNCTION DERIVATIVES

FOR THE LINEAR INTERPOLATION FUNCTIONS: these are used to interpolate the concentration derivatives; multiplication by the inverse Jacobian converts the local derivatives into global derivatives:

$$\frac{dg_1(r)}{dr} \equiv -\frac{1}{2}$$
$$\frac{dg_2(r)}{dr} \equiv +\frac{1}{2}$$

These interpolation function derivatives do not depend explicitly on the local coordinate, r, but function definitions are maintained as a reminder of the implied dependence on local coordinate.

FOR THE QUADRATIC INTERPOLATION FUNCTIONS: these are used to interpolate displacement derivatives; multiplication by the inverse Jacobian converts the local derivatives into global derivatives:

$$\frac{dh_1(r)}{dr} \equiv \left(r - \frac{1}{2}\right)$$
$$\frac{dh_2(r)}{dr} \equiv -2r$$
$$\frac{dh_3(r)}{dr} \equiv \left(r + \frac{1}{2}\right)$$

```
C
C     DISTRIBUTED LOAD SPECIFICATION ROUTINE
C
      subroutine KFCALC(JDLTYP,F,XGAUS,TTIME)
      double precision F(*),XGAUS(*),TTIME
      integer JDLTYP
      double precision A,EPS

C     THIS LOAD ROUTINE CALCULATES THE BODY FORCE AT THE
C     GAUSS POINTS FOR USE IN FINDING THE RHS VECTOR


      IF(JDLTYP.EQ.-1) THEN
C
C        LOAD TYPE 1 INDICATES A DISTRIBUTED BODY FORCE OF THE FORM
C           F(X)= A/(X+EPS)^3/2
C        GRAVITATIONAL BODY FORCE FOR 4340 STEEL IS ~80.0D3 [N/m^3]
C        'A' SHOULD BE SPECIFIED IN UNITS OF [FORCE/LENGTH^3/2]

         A=15.0D6
         EPS=1.0D-18
         DO 100 I=1,2
  100     F(I)=A/sqrt((abs(XGAUS(I))+EPS)**3.0D0)

      ENDIF


      return
      end
```


DISTRIBUTED LOAD SPECIFICATION ROUTINE returns a load value at the global Gauss point locations from an user-defined non-uniform load distribution. The coding in the present case is for a singular body force applied as a function of the global coordinate x. The value of the load at the i^{th} Gauss point is returned to UEL as `F(i)`. The subroutine receives the current distributed load type, `JDLTYP`, the global Gauss point coordinates, and the total time completed in the analysis.

Several different non-uniformly distributed load functions may be evaluated by adding `IF` statements to flag on the values of `JDLTYP`. These loads may be functions of the global location coordinate, x, and current analysis time, t. If additional load functions are to be added, they should follow the format of the load function given here, so that one load value is returned for each Gauss point on the element.

In steady-state analyses, a "time" is defined and used to indicate the fraction of analysis completed. This allows for the gradual application of a distributed load in order to avoid potential numerical difficulties. See `TIME` in AUM (II; 5.2.16-7) for additional information.

NOTE ON CONSISTENT NODAL LOADINGS: UEL converts the distributed loads to consistent nodal loads by integration of the product of the quadratic displacement interpolation function and the distributed load over the length of the element. For example, on the first node, the consistent nodal load, P, would be

$$P = A_e \int_{-1}^{+1} \{h_1(r)\} F_x(r) |\, J \,| dr$$

which when evaluated via Gaussian integration gives:

$$P = W_1 A_e \{h_1(r_1)\} F_x(r_1) |\, J(r_1) \,| + W_2 A_e \{h_1(r_2)\} F_x(r_2) |\, J(r_2) \,|$$

where r_i and W_i are the Gauss locations and weights respectively. Since `subroutine KFCALC` returns the values of the load function at the Gauss points, $F_x(r_i)$, this evaluation becomes trivial.

APPENDIX C: Sample Input Deck

This Appendix contains a copies of the ABAQUS input decks that were used to solve the Case 1a, 2a, and 3a problems. A section-by-section annotated listing is also included.

ABAQUS Input Deck: Case 1a

```
*HEADING, UNSYMM
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
**      C(0)=0.0                          C(L)=1E-6
**     //
**     //---------------------------------------- F(x)=0
**     //
**       U(0)=0.0                          t(L)=0.0
**
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*PREPRINT
*NODE, NSET=ROD
1,0.0D0
21,0.10D0
*NGEN,NSET=ROD
1,21,1
*USER ELEMENT, NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
** THE FIRST AND THIRD NODES HAVE DEGREES OF FREEDOM IN CONCENTRATION AND
** DISPLACMENT, WHILE THE SECOND NODE ONLY HAS DISPLACEMENT DEGREES OF
** FREEDOM.  NOTE THAT CONCENTRATIONS ARE TREATED AS TEMPERATURE D.O.F.
11,1
2,1
3,11,1
*ELEMENT,TYPE=U1,ELSET=SC1D
1,1,2,3
*ELGEN, ELSET=SC1D
1,10,2,1,1,1,1,1
*UEL PROPERTY, ELSET=SC1D
** PROPERTIES ARE IN THE ORDER:
** CFLAG,AREA,E,NU,D,ALPHA,CREF,RHO,
** MW,TEMP,TRAPS
1.0D0,1.0D-4,200.0D9,0.3D0,1.0D-9,5.2D0,0.0D0,7.8D3,
1.00797D-3,293.0D0,19.0D0
*MATERIAL,NAME=A4340
*DEPVAR
9
*BOUNDARY
** ZERO DISPLACEMENT AT LHS
1,1
** ZERO CONCENTRATION AT LHS
1,11
*INITIAL CONDITIONS, TYPE=TEMPERATURE
** 0.0 INITIAL CONCENTRATION OVER ROD LENGTH
ROD,0.0D0
*WAVEFRONT MINIMIZATION, SUPPRESS
*STEP,INC=1000
*COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
0.005,1.0, ,0.05
**
*CONTROLS, PARAMETERS=FIELD,FIELD=TEMPERATURE
 , ,5.0D-21
**
*NODE PRINT, SUMMARY=NO,FREQUENCY=100
COOR1,U1,NT
*EL PRINT, SUMMARY=NO,FREQUENCY=100
SDV
*BOUNDARY
** SPECIFY RIGHT HAND BOUNDARY CONCENTRATION AS 1.0E-6
21,11,11,1.0D-6
*END STEP
```

ABAQUS Input Deck: Case 2a

```
*HEADING, UNSYMM
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 2
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
**       C(0)=0.0                          C(L)=1E-6
**     //                                    //
**     //--------------------------------------//  F(x)=0
**     //                                    //
**       U(0)=0.0                          U(L)=0.0
**
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*PREPRINT
*NODE, NSET=ROD
1,0.0D0
21,0.10D0
*NGEN,NSET=ROD
1,21,1
*USER ELEMENT, NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
** THE FIRST AND THIRD NODES HAVE DEGREES OF FREEDOM IN CONCENTRATION AND
** DISPLACMENT, WHILE THE SECOND NODE ONLY HAS DISPLACEMENT DEGREES OF
** FREEDOM.  NOTE THAT CONCENTRATIONS ARE TREATED AS TEMPERATURE D.O.F.
11,1
2,1
3,11,1
*ELEMENT,TYPE=U1,ELSET=SC1D
1,1,2,3
*ELGEN, ELSET=SC1D
1,10,2,1,1,1,1,1
*UEL PROPERTY, ELSET=SC1D
** PROPERTIES ARE IN THE ORDER:
** CFLAG,AREA,E,NU,D,ALPHA,CREF,RHO
** MW,TEMP,TRAPS
1.0D0,1.0D-4,200.0D9,0.3D0,1.0D-9,5.2D0,0.0D0,7.8D3,
1.00797D-3,293.0D0,19.0D0
*MATERIAL,NAME=A4340
*DEPVAR
9
*BOUNDARY
** ZERO DISPLACEMENT AT LHS
1,1
** ZERO DISPLACEMENT AT RHS
21,1
** ZERO CONCENTRATION AT LHS
1,11
*INITIAL CONDITIONS, TYPE=TEMPERATURE
** 0.0 INITIAL CONCENTRATION OVER ROD LENGTH
ROD,0.0D0
*WAVEFRONT MINIMIZATION, SUPPRESS
*STEP,INC=1000
*COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
0.005,1.0, ,0.05
**
*CONTROLS, PARAMETERS=FIELD,FIELD=TEMPERATURE
 , ,5.0D-21
**
*NODE PRINT, SUMMARY=NO,FREQUENCY=100
COOR1,U1,NT
*EL PRINT, SUMMARY=NO,FREQUENCY=100
SDV
*BOUNDARY
** SPECIFY RIGHT HAND BOUNDARY CONCENTRATION AS 1.0E-6
21,11,11,1.0D-6
*END STEP
```

ABAQUS Input Deck: Case 3a (Low Trapping)

```
*HEADING, UNSYMM
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 3 (200 elements) LOW TRAPPING
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
**      J(4.0E-5)=0.0                    C(L)=1E-7
**     //
**     //---------------------------------          F(x)=15E6/(x+eps)^(3/2)
**     //
**       U(4.0E-5)=0.0
**
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*PREPRINT
*NODE, NSET=A
1,4.0D-5
**
*NODE,NSET=B
401,0.10D0
**
*NFILL,NSET=ROD,BIAS=9.470049D-1,TWO STEP
A,B,400,1
**
*USER ELEMENT, NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
** THE FIRST AND THIRD NODES HAVE DEGREES OF FREEDOM IN CONCENTRATION AND
** DISPLACMENT, WHILE THE SECOND NODE ONLY HAS DISPLACEMENT DEGREES OF
** FREEDOM.  NOTE THAT CONCENTRATIONS ARE TREATED AS TEMPERATURE D.O.F.
11,1
2,1
3,11,1
**
*ELEMENT,TYPE=U1,ELSET=SC1D
1,1,2,3
*ELGEN, ELSET=SC1D
1,200,2,1,1,1,1,1
*UEL PROPERTY, ELSET=SC1D
** PROPERTIES ARE IN THE ORDER:
** CFLAG,AREA,E,NU,D,ALPHA,CREF,RHO
** MW,TEMP,TRAPS
1.0D0,1.0D-4,200.0D9,0.3D0,1.0D-9,5.2D0,0.0D0,7.8D3
1.00797D-3,293.0D0,19.0D0
*MATERIAL,NAME=A4340
*DEPVAR
9
*BOUNDARY
** ZERO DISPLACEMENT AT LHS
1,1
*INITIAL CONDITIONS, TYPE=TEMPERATURE
** 1.0E-7 INITIAL CONCENTRATION OVER ROD LENGTH
ROD,1.0D-7
**
*WAVEFRONT MINIMIZATION, SUPPRESS
*STEP,INC=5000,AMPLITUDE=STEP
*COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
1.0D-4,1.0, ,5.0D-3
**
*CONTROLS, PARAMETERS=FIELD,FIELD=TEMPERATURE
 , ,5.0D-21
**
*DLOAD,OP=NEW
SC1D,U1NU
**
*NODE PRINT, SUMMARY=NO, FREQUENCY=100
COOR1,U1,NT
*EL PRINT, SUMMARY=NO, FREQUENCY=100
SDV
**
*BOUNDARY
** SPECIFY RIGHT HAND BOUNDARY CONCENTRATION AS 1.0E-7
401,11,11,1.0D-7
*END STEP
```

ABAQUS Input Deck: Case 3a (High Trapping)

```
*HEADING, UNSYMM
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 3 (200 elements)HIGH TRAPPING
** * * *
```

```
*HEADING, UNSYMM
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 3 (200 elements)
```

```
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
**       J(04.0E-5)=0.0                    C(L)=1E-7
**     //
**     //----------------------------- <== P[N]      F(x)=15E6/(x+eps)^(3/2)
**     //
**       U(4.0E-5)=0.0
**
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*PREPRINT
```


Sample Input Deck

As with the notes on the User Element, these notes are complied for a user who is familiar with the typical components of an ABAQUS input deck. Explanations are primarily given for specific elements of the input deck which apply to User Elements in general or the Fully-Coupled Solute-Solid mixture theory in particular. Details concerning input deck command formats may be found in ABAQUS User's Manual II.

The sample input deck illustrates values typical of a steady-state coupled solute transport problem. The deck presented here is intended to demonstrate a variety of analysis options and their applications to the UEL routine. The problem geometry for this case is a $10\,cm$ long rod modeled using 200 finite elements with the specified boundary conditions:

Concentration Boundary Conditions $\begin{cases} \mathcal{J}(4.0 \times 10^{-5}\,[m]) = 0.0\,[m(gH/gFe)/s] \\ c(0.1\,[m]) = 10^{-7}[gH/gFe] \end{cases}$

Momentum Boundary Conditions $\begin{cases} u(4.0 \times 10^{-5}\,[m]) = 0.0\,[m] \\ P(0.1\,[m]) = -1000\,[N] \end{cases}$

Body Force: $F_x = \dfrac{15 \times 10^6}{\sqrt{(x+\epsilon)^3}}\,[N/m^3]$

Initial Concentration Distribution: $c(x) = 10^{-7}[gH/gFe]$

All of the property values are specified in SI basic units (kg,m,s), though any dimensionally consistent set of units can be used. All non-integer numerical values are entered using the double-precision format.

```
*NODE, NSET=A
1,4.0D-5
**
*NODE,NSET=B
401,0.10D0
**
```

NODE ASSIGNMENT follows standard ABAQUS conventions. Certain peculiarities arise in this problem which require care in the node selection process. The singular body force problem exhibits multi-valued solutions for the concentration as the singularity is approached. If one tries to use ABAQUS to solve the problem in this region, warnings for negative eigenvalues will be returned. Two remedies exist for this problem, but both require an analytical solution for the problem. The user may restrict the region of the model to the well behaved portion of the solution domain, as is done here by establishing the left-hand side of the model at $x = 4.0 \times 10^{-5}$ [m]; or the body force function may be altered so that the rod starts at $x = 0$ [m] but the singularity of the body force occurs at a point $x_s < 0$:

$$F_x = \frac{15 \times 10^6}{\sqrt{(x + ||x_s||)^3}}$$

```
*NFILL,NSET=ROD,BIAS=9.470049D-1,TWO STEP
A,B,400,1
**
```

NODAL GENERATION with biasing requires the use of the "two-step" parameter since the elements are three-noded and this places the internal node at the center of each undeformed element (see AUM (II; 9.4.5-1) for further explanation of biasing). To allow comparison between models with different numbers of elements, the bias has been selected so that the ratio of the lengths of the largest to smallest element in a model remain constant. Using this constraint, the bias of an n element model may be calculated as:

$$b_n = (b_N)^{\frac{N-1}{n-1}}$$

where N represents the number of elements in the "benchmark" model. The benchmark selected for this problem was a 10 element model with bias, $b_{10} = 0.3$.


```
*USER ELEMENT,
NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
** THE FIRST AND THIRD NODES HAVE DEGREES OF FREEDOM IN CONCENTRATION AND
** DISPLACMENT, WHILE THE SECOND NODE ONLY HAS DISPLACEMENT DEGREES OF
** FREEDOM.  NOTE THAT CONCENTRATIONS ARE TREATED AS TEMPERATURE D.O.F.
11,1
2,1
3,11,1
```

User Element Declaration should be entered into the input deck exactly as shown here for use with the 1-D Coupled Deformation-Diffusion user element. Since the current coding of the UEL subroutine does not check for element type, the *TYPE* declaration is arbitrary as long as it corresponds to the *TYPE* parameter in the element definition. If the user wishes to study a model with more than one User Element type, coding must be added to the User Element to check this parameter, as specified in AUM (II; 5.2.16-7).

The degrees of freedom on the element are specified according to ABAQUS conventions as

$$\lfloor U(1), U(2), U(3), U(4), U(5) \rfloor = \lfloor c_1, u_1, u_2, c_2, u_3 \rfloor$$

The ABAQUS analysis type is "Coupled Temperature-Displacement, Steady-State", so the nodal concentrations, c_i, are specified as nodal temperatures.

```
*ELEMENT,TYPE=U1,ELSET=SC1D
1,1,2,3
*ELGEN, ELSET=SC1D
1,200,2,1,1,1,1,1

*UEL PROPERTY, ELSET=SC1D
** PROPERTIES ARE IN THE ORDER:
** KFLAG,AREA,E,NU,D,ALPHA,CREF,RHO
** MW,TEMP,TRAPS
1.0D0,1.0D-4,200.0D9,0.3D0,1.0D-9,5.2D0,0.0D0,7.8D3
1.00797D-3,293.0D0,499.0D0
```



```
*MATERIAL,NAME=A4340
*DEPVAR
9

*BOUNDARY
** ZERO DISPLACEMENT AT LHS
1,1

*INITIAL CONDITIONS, TYPE=TEMPERATURE
** 1.0E-7 INITIAL CONCENTRATION OVER ROD LENGTH
ROD,1.0D-7
```

ELEMENT DEFINITION follows standard ABAQUS conventions. The *TYPE* specification must be identical to the type specification in the *USER ELEMENT* command.

USER ELEMENT PROPERTIES are used to specify a particular analysis and the physical properties of the mixture. The physical properties are currently assumed to be constants. All values must be entered in double-precision format, including the analysis case flag, KFLAG. The required property specifications are defined below, and they must be entered in the given order, with 8 properties in the first line and 3 in the second, as specified by ABAQUS.

1. **KFLAG**[1] = variable used to indicate the degree of coupling and the type of linear elastic constitutive behavior.
   KFLAG values: 1 ⇒ Plane Stress, Fully Coupled
   2 ⇒ Plane Strain, Fully Coupled
   3 ⇒ Plane Stress, Weakly Coupled
   4 ⇒ Plane Strain, Weakly Coupled
2. **AREA** ≡ cross-sectional area $[m^2]$.
3. **E** ≡ modulus of elasticity $[Pa]$.
4. **NU** ≡ Poisson's ratio [1].
5. **D** ≡ diffusion coefficient $[m^2/s]$.
6. **ALPHA** ≡ linear expansion coefficient for the solute = $\frac{1}{3}\frac{\rho}{\mathcal{M}_S}\overline{V}_S$ $[m/m/\Delta c_S]$.
7. **CREF** ≡ reference solute concentration (i.e., c_o term in $\Delta c = c - c_o$) $[gSol/gMix]$
8. **RHO** ≡ density ($\simeq \rho_{\text{Solid}}$) $[kg/m^3]$.
9. **MW** ≡ molecular weight of solute species $[kg/mol]$.
10. **TEMP** ≡ temperature $[K]$.
11. **TRAPS**[2] ≡ reversible trap site constant (i.e., $c_R^s K_R$) [1].

MATERIAL DEFINITION must be included to allow for the *DEPVAR sub option, which allows printout of the state variables calculated in the User Element. The name assigned to the material is arbitrary, since no material properties are included through this command.

ZERO BOUNDARY CONDITIONS are specified according to ABAQUS convention.

INITIAL CONDITIONS are specified according to ABAQUS convention.

---

[1] To run a case with no coupling (i.e. standard linear elasticity combined with classical diffusion) the parameter ALPHA must be set equal to zero. KFLAG is then used to select plane-stress or plane-strain analysis; changing between "Fully-Coupled" and "Weakly-Coupled" analysis will have no effect.

[2] For the hydrogen in steels, the term $(1 + c_R^s K_R)$ is assumed to be in the range of 1 to 500, yielding a range in the TRAPS variable of 0 to 499.

```
*WAVEFRONT MINIMIZATION, SUPPRESS
```

WAVEFRONT MINIMIZATION can be suppressed, since it is seldom needed in 1-D problems in which the element and node numbering begins at one end of the rod and continues along consecutively.

```
*STEP,INC=5000,AMPLITUDE=STEP
```

BEGIN ANALYSIS STEP

```
*COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
2.0D-4,1.0D5,2.0D-10,1.0D3
```

COUPLED TEMPERATURE-DISPLACEMENT analysis is used in conjunction with the User Element, with mass-fraction concentrations replacing the temperature degrees of freedom in the analysis.

```
*CONTROLS, PARAMETERS=FIELD,FIELD=TEMPERATURE
5.0D-3,,5.0D-21
```

CONTROLS for solution convergence must be set for the concentration (temperature) field because the magnitude of the concentration flux is much smaller than the magnitude of the stress flux, and a single criterion for both does not work very well. The steady state concentration flux for problems with concentrations of 10^{-7} specified at one end of the rod and 0 at the other end is on the order of 10^{-15}, so specifying the initial control at 10^{-21} represents an essentially zero flux residual.

```
*DLOAD,OP=NEW
SC1D,U1NU
```

DISTRIBUTED LOAD definition allows for the addition of body forces to the User Element model. ABAQUS defines two types of distributed loads in a User Element: Un and $UnNU$. Load type Un is independent of local or global position on the element, but may vary with time using `*AMPLITUDE` definition. Type $UnNU$ may be defined (in the UEL subroutine) as a function of the global coordinates and time.

All $UnNU$ type loads are defined in the `subroutine FCALC` in our user element coding. At present, the only $UnNU$ load in `subroutine FCALC` is $U1NU$ which corresponds to a singular body force of the form:

$$F_x = \frac{A}{\sqrt{(x+\epsilon)^3}} \left[\frac{N}{m^3}\right]$$

where A and ϵ are set within `subroutine FCALC`. ϵ is used to prevent a numerically unstable situation at $x = 0$. Additional load functions may be added by following the current format in `subroutine FCALC`.

```
*CLOAD,OP=NEW
B,1,-1.0D3
```

CONCENTRATED LOADS Distributed surface tractions are included in the model by calculating the corresponding consistent nodal loads and entering these in the concentrated load option, `*CLOAD`. These loads should be entered in using the proper ABAQUS format.

```
*NODE PRINT, SUMMARY=NO, FREQUENCY=100
COOR1,U1,NT


*EL PRINT, SUMMARY=NO, FREQUENCY=100
SDV
```

OUTPUT SPECIFICATION follows ABAQUS conventions. The `*NODE PRINT` option requests ABAQUS to print the nodal displacements in the axial direction ($U1$) and the nodal temperatures (NT, which, in this case, are actually the concentrations). The `*EL PRINT` request prints the state variables of the model under the output heading $SDVi$ ($i = 1...9$). These labels correspond to:

SDV1 $\equiv$ Dilatational strain, e, at the left-hand integration point on the element $[m/m]$.
SDV2 $\equiv$ Dilatational strain, e, at the right-hand integration point on the element $[m/m]$.
SDV3 $\equiv$ Axial stress, σ_x, at the left-hand integration point on the element $[Pa]$.
SDV4 $\equiv$ Axial stress, σ_x, at the right-hand integration point on the element $[Pa]$.
SDV5 $\equiv$ Approximate axial stress, σ_x, at the left-hand end of the element $[Pa]$.
SDV6 $\equiv$ Approximate axial stress, σ_x, at the right-hand end of the element $[Pa]$.
SDV7 $\equiv$ Mass flux at the center of each element $[m(gH/gFe)/s]$.
SDV8 $\equiv$ Global coordinate of left-hand integration point (for plotting $SDV1\&3$) $[m]$.
SDV9 $\equiv$ Global coordinate of right-hand integration point (for plotting $SDV2\&4$) $[m]$.

```
*BOUNDARY
** SPECIFY RIGHT HAND BOUNDARY CONCENTRATION AS 1.0E-7
401,11,11,1.0D-7


*END STEP
```

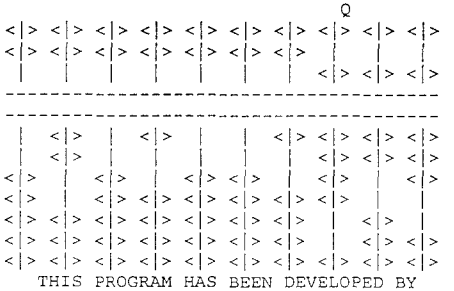
NON-ZERO BOUNDARY CONDITIONS are entered and applied according to standard ABAQUS conventions.

END ANALYSIS STEP

APPENDIX D: Sample Output

This Appendix contains a copy of an ABAQUS output listing generated in the solution of a 1-D fully coupled deformation-diffusion problem.

```
  AAAAAA     BBBBBBBBB      AAAAAA      QQQQQQQQ    U        U    SSSSSSSS
 A      A    B        B    A      A    Q        Q   U        U   S
A        A   B        B   A        A   Q        Q   U        U   S
A        A   B        B   A        A   Q        Q   U        U   S
AAAAAAAAAA   BBBBBBBBB    AAAAAAAAAA   Q        Q   U        U    SSSSSSSS
A        A   B        B   A        A   Q    Q   Q   U        U            S
A        A   B        B   A        A   Q     Q  Q   U        U            S
A        A   B        B   A        A   Q      Q Q   U        U            S
A        A   BBBBBBBBB    A        A    QQQQQQQQ     UUUUUUUU     SSSSSSSS
                                                  Q
```



```
   THIS PROGRAM HAS BEEN DEVELOPED BY
HIBBITT, KARLSSON AND SORENSEN, INC.
        1080 MAIN STREET
     PAWTUCKET, R.I. 02860
```

THIS IS A PROPRIETARY PROGRAM AND IS MADE AVAILABLE
FOR INTERNAL USE AT UNIVERSITY OF NOTRE DAME,
UNDER THE TERMS OF THE ACADEMIC LICENSE AGREEMENT
WITH H.K.S. ALL USAGE MUST BE UNDER THE DIRECT
SUPERVISION AND CONTROL OF THE DESIGNATED USER.
THE DESIGNATED USER IS PAUL GO.
ANY NON-ACADEMIC USAGE OF THE PROGRAM REQUIRES
PAYMENT OF A MONTHLY CHARGE. ASSISTANCE AND
OTHER INFORMATION MAY BE OBTAINED FROM THE
DESIGNATED USER.

ON MACHINE 8035E88D,
YOU ARE AUTHORIZED TO RUN
STANDARD, AQUA, AND POST UNTIL 11/30/95
YOUR SITE ID IS: U. NOTRE DAME

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*                                                                       *
*                    ****************                                   *
*                    * N O T I C E  *                                   *
*                    ****************                                   *
*                                                                       *
*                                                                       *
*                 THIS IS ABAQUS VERSION 5.3.                           *
*                                                                       *
*                                                                       *
*  PLEASE MAKE SURE YOU ARE USING VERSION 5.3 MANUALS                   *
*  PLUS THE NOTES ACCOMPANYING THIS RELEASE. THESE NOTES                *
*  CAN BE OBTAINED BY USING THE INFORMATION OPTION ON THE               *
*  ABAQUS COMMAND LINE.                                                 *
*                                                                       *
*                                                                       *
*   THIS PROGRAM MAY NOT BE USED FOR COMMERCIAL PURPOSES                *
*           WITHOUT PAYMENT OF A MONTHLY CHARGE.                        *
*                                                                       *
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
```

A B A Q U S I N P U T E C H O

```
     5   10   15   20   25   30   35   40   45   50   55   60   65   70   75   80
----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
*HEADING, UNSYMM
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
**   C(0)=0.0                          C(L)=1E-6
**    //
**    //---------------------------------------- F(x)=0
**    //
**   U(0)=0.0                          t(L)=0.0
**
** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*PREPRINT
*NODE, NSET=ROD
1,0.0D0
21,0.10D0
*NGEN,NSET=ROD
1,21,1
*USER ELEMENT, NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
** THE FIRST AND THIRD NODES HAVE DEGREES OF FREEDOM IN CONCENTRATION AND
** DISPLACMENT, WHILE THE SECOND NODE ONLY HAS DISPLACEMENT DEGREES OF
** FREEDOM.  NOTE THAT CONCENTRATIONS ARE TREATED AS TEMPERATURE D.O.F.
11,1
2,1
3,11,1
*ELEMENT,TYPE=U1,ELSET=SC1D
1,1,2,3
*ELGEN, ELSET=SC1D
1,10,2,1,1,1,1,1
*UEL PROPERTY, ELSET=SC1D
** PROPERTIES ARE IN THE ORDER:
** CFLAG,AREA,E,NU,D,ALPHA,CREF,RHO,
** MW,TEMP,TRAPS
1.0D0,1.0D-4,200.0D9,0.3D0,1.0D-9,5.2D0,0.0D0,7.8D3,
1.00797D-3,293.0D0,19.0D0
*MATERIAL,NAME=A4340
*DEPVAR
9
*BOUNDARY
** ZERO DISPLACEMENT AT LHS
1,1
** ZERO CONCENTRATION AT LHS
----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
     5   10   15   20   25   30   35   40   45   50   55   60   65   70   75   80
```

```
                    5   10   15   20   25   30   35   40   45   50   55   60   65   70   75   80
                    ----------------------------------------------------------------------------
                    1,11
                    *INITIAL CONDITIONS, TYPE=TEMPERATURE
                    ** 0.0 INITIAL CONCENTRATION OVER ROD LENGTH
                    ROD,0.0D0
  CARD    45        *WAVEFRONT MINIMIZATION, SUPPRESS
                    *STEP,INC=1000
                    *COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
                    0.005,1.0, , 0.05
                    **
  CARD    50        *CONTROLS, PARAMETERS=FIELD,FIELD=TEMPERATURE
                     , ,5.0D-21
                    **
                    *NODE PRINT, SUMMARY=NO,FREQUENCY=100
                    COOR1,U1,NT
  CARD    55        *EL PRINT, SUMMARY=NO,FREQUENCY=100
                    SDV
                    *BOUNDARY
                    ** SPECIFY RIGHT HAND BOUNDARY CONCENTRATION AS 1.0E-6
                    21,11,11,1.0D-6
  CARD    60        *END STEP

                    ----------------------------------------------------------------------------
                    5   10   15   20   25   30   35   40   45   50   55   60   65   70   75   80
                    ----------------------------------------------------------------------------
   OPTIONS BEING PROCESSED
 ***************************
*HEADING, UNSYMM
       STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1
*NODE, NSET=ROD
*NGEN,NSET=ROD
*USER ELEMENT, NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
*ELEMENT,TYPE=U1,ELSET=SC1D
*ELGEN, ELSET=SC1D
*MATERIAL,NAME=A4340
*DEPVAR
*DEPVAR
*USER ELEMENT, NODES=3,UNSYMM,COORDINATES=1,PROPERTIES=11,VARIABLES=9,TYPE=U1
*UEL PROPERTY, ELSET=SC1D
*INITIAL CONDITIONS, TYPE=TEMPERATURE
*INITIAL CONDITIONS, TYPE=TEMPERATURE
*STEP,INC=1000
*COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
*CONTROLS, PARAMETERS=FIELD,FIELD=TEMPERATURE
*EL PRINT, SUMMARY=NO,FREQUENCY=100
```

FOR USE AT UNIVERSITY OF NOTRE DAME UNDER ACADEMIC LICENSE FROM HKS, INC.
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1

```
*BOUNDARY
*END STEP
*BOUNDARY
*STEP,INC=1000
*COUPLED TEMPERATURE-DISPLACEMENT, STEADY STATE
*NODE PRINT, SUMMARY=NO,FREQUENCY=100
*BOUNDARY
*END STEP
```

FOR USE AT UNIVERSITY OF NOTRE DAME UNDER ACADEMIC LICENSE FROM HKS, INC.
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1

E L E M E N T D E F I N I T I O N S

NUMBER	TYPE	PROPERTY REFERENCE	NODES FORMING ELEMENT		
1	U1	1	1	2	3
2	U1	1	3	4	5
3	U1	1	5	6	7
4	U1	1	7	8	9
5	U1	1	9	10	11
6	U1	1	11	12	13
7	U1	1	13	14	15
8	U1	1	15	16	17
9	U1	1	17	18	19
10	U1	1	19	20	21

U S E R E L E M E N T S

ELEMENT TYPE U1
NUMBER OF NODES 3
NUMBER OF COORDINATES 1
NUMBER OF PROPERTIES 11
NUMBER OF VARIABLES 9
UNSYMMETRIC ELEMENT
DEGREES OF FREEDOM

NODE	D.O.F.
1	11 1
2	1
3	11 1

U S E R E L E M E N T P R O P E R T Y

PROPERTY NUMBER 1

PROPERTIES	1.000	1.0000E-04	2.0000E+11	0.3000	1.0000E-09	5.200	0.	7800.
	1.0080E-03	293.0	19.00	0.	0.	0.	0.	0.

M A T E R I A L D E S C R I P T I O N

MATERIAL NAME: A4340

NUMBER OF SOLUTION DEPENDENT STATE VARIABLES IS 9

E L E M E N T S E T S

SET	SC1D	MEMBERS	1	2	3	4	5	6	7	8	9	10

N O D E S E T S

SET	ROD	MEMBERS	1	2	3	4	5	6	7	8	9	10	11	12
			13	14	15	16	17	18	19	20	21			

N O D E D E F I N I T I O N S

NODE NUMBER	COORDINATES			SINGLE POINT CONSTRAINTS TYPE	PLUS	DOF
1	0.	0.	0.		1	11
2	5.00000E-03	0.	0.			
3	1.00000E-02	0.	0.			

STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1

4	1.50000E-02	0.	0.
5	2.00000E-02	0.	0.
6	2.50000E-02	0.	0.
7	3.00000E-02	0.	0.
8	3.50000E-02	0.	0.
9	4.00000E-02	0.	0.
10	4.50000E-02	0.	0.
11	5.00000E-02	0.	0.
12	5.50000E-02	0.	0.
13	6.00000E-02	0.	0.
14	6.50000E-02	0.	0.
15	7.00000E-02	0.	0.
16	7.50000E-02	0.	0.
17	8.00000E-02	0.	0.
18	8.50000E-02	0.	0.
19	9.00000E-02	0.	0.
20	9.50000E-02	0.	0.
21	0.10000	0.	0.

S T E P 1 C O U P L E D - T E M P E R A T U R E - D I S P L A C E M E N T A N A L Y S I S

STEADY STATE ANALYSIS

AUTOMATIC TIME CONTROL WITH -
A SUGGESTED INITIAL TIME INCREMENT OF 5.000E-03
AND A TOTAL TIME PERIOD OF 1.00
THE MINIMUM TIME INCREMENT ALLOWED IS 1.000E-05
THE MAXIMUM TIME INCREMENT ALLOWED IS 5.000E-02
CREEP AND SWELLING EFFECTS ARE OMITTED IN THIS STEP

CONVERGENCE TOLERANCE PARAMETERS FOR FORCE

CRITERION FOR RESIDUAL FORCE FOR A NONLINEAR PROBLEM	5.000E-03
CRITERION FOR DISP. CORRECTION IN A NONLINEAR PROBLEM	1.000E-02
INITIAL VALUE OF TIME AVERAGE FORCE	1.000E-02
AVERAGE FORCE IS TIME AVERAGE FORCE	
ALTERNATE CRIT. FOR RESIDUAL FORCE FOR A NONLINEAR PROBLEM	2.000E-02
CRITERION FOR ZERO FORCE RELATIVE TO TIME AVRG. FORCE	1.000E-05
CRITERION FOR DISP. CORRECTION IN A LINEAR PROBLEM	1.000E-03
CRITERION FOR RESIDUAL FORCE FOR A LINEAR PROBLEM	1.000E-08
FIELD CONVERSION RATIO	1.00

CONVERGENCE TOLERANCE PARAMETERS FOR HEAT FLUX

CRITERION FOR RESIDUAL HEAT FLUX FOR A NONLINEAR PROBLEM	5.000E-03
CRITERION FOR TEMP. CORRECTION IN A NONLINEAR PROBLEM	1.000E-02
*** INITIAL VALUE OF TIME AVERAGE HEAT FLUX	5.000E-21
AVERAGE HEAT FLUX IS TIME AVERAGE HEAT FLUX	
ALTERNATE CRIT. FOR RESIDUAL HEAT FLUX FOR A NONLINEAR PROBLEM	2.000E-02
CRITERION FOR ZERO HEAT FLUX RELATIVE TO TIME AVRG. HEAT FLUX	1.000E-05
CRITERION FOR TEMP. CORRECTION IN A LINEAR PROBLEM	1.000E-03
CRITERION FOR RESIDUAL HEAT FLUX FOR A LINEAR PROBLEM	1.000E-08

FOR USE AT UNIVERSITY OF NOTRE DAME UNDER ACADEMIC LICENSE FROM HKS, INC.

STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1

FIELD CONVERSION RATIO	1.00
VOLUMETRIC STRAIN COMPATIBILITY TOLERANCE FOR HYBRID SOLIDS	1.000E-05
AXIAL STRAIN COMPATIBILITY TOLERANCE FOR HYBRID BEAMS	1.000E-05
TRANS. SHEAR STRAIN COMPATIBILITY TOLERANCE FOR HYBRID BEAMS	1.000E-05
SOFT CONTACT CONSTRAINT COMPATIBILITY TOLERANCE	5.000E-03

*** INDICATES USE OF NON-DEFAULT CONVERGENCE TOLERANCE PARAMETER
SELECTED WITH *CONTROLS

TIME INCREMENTATION CONTROL PARAMETERS:

FIRST EQUILIBRIUM ITERATION FOR CONSECUTIVE DIVERGENCE CHECK	4
EQUILIBRIUM ITERATION AT WHICH LOG. CONVERGENCE RATE CHECK BEGINS	8
EQUILIBRIUM ITERATION AFTER WHICH ALTERNATE RESIDUAL IS USED	9
MAXIMUM EQUILIBRIUM ITERATIONS ALLOWED	16
EQUILIBRIUM ITERATION COUNT FOR CUT-BACK IN NEXT INCREMENT	10
MAXIMUM EQUILIB. ITERS IN TWO INCREMENTS FOR TIME INCREMENT INCREASE	4
MAXIMUM ITERATIONS FOR SEVERE DISCONTINUITIES	12
MAXIMUM CUT-BACKS ALLOWED IN AN INCREMENT	5
MAXIMUM DISCON. ITERS IN TWO INCREMENTS FOR TIME INCREMENT INCREASE	6
CUT-BACK FACTOR AFTER DIVERGENCE	0.2500
CUT-BACK FACTOR FOR TOO SLOW CONVERGENCE	0.5000
CUT-BACK FACTOR AFTER TOO MANY EQUILIBRIUM ITERATIONS	0.7500
CUT-BACK FACTOR AFTER TOO MANY SEVERE DISCONTINUITY ITERATIONS	0.2500
CUT-BACK FACTOR AFTER PROBLEMS IN ELEMENT ASSEMBLY	0.2500
INCREASE FACTOR AFTER TWO INCREMENTS THAT CONVERGE QUICKLY	1.500
MAX. TIME INCREMENT INCREASE FACTOR ALLOWED	1.500
MAX. TIME INCREMENT INCREASE FACTOR ALLOWED (DYNAMICS)	1.250
MAX. TIME INCREMENT INCREASE FACTOR ALLOWED (DIFFUSION)	2.000
MINIMUM TIME INCREMENT RATIO FOR EXTRAPOLATION TO OCCUR	0.1000
MAX. RATIO OF TIME INCREMENT TO STABILITY LIMIT	1.000
FRACTION OF STABILITY LIMIT FOR NEW TIME INCREMENT	0.9500
THE MAXIMUM NUMBER OF INCREMENTS IN THIS STEP IS	1000

EXTRAPOLATION WILL BE USED

PRINT OF INCREMENT NUMBER, TIME, ETC., EVERY 1 INCREMENTS

FOR USE AT UNIVERSITY OF NOTRE DAME UNDER ACADEMIC LICENSE FROM HKS, INC.
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1

E L E M E N T P R I N T

THE FOLLOWING TABLE IS PRINTED FOR ALL ELEMENTS WITH TYPE U1 AT EVERY 100 INCREMENT AT THE INTEGRATION POINTS

TABLE	1	SDV1	SDV2	SDV3	SDV4	SDV5	SDV6	SDV7	SDV8	SDV9

N O D E P R I N T

THE FOLLOWING TABLE IS PRINTED FOR ALL NODES AT EVERY 100 INCREMENT

TABLE	1	COOR1	U1	NT11

B O U N D A R Y C O N D I T I O N S

NODE	DOF	AMP. REF.	MAGNITUDE	NODE	DOF	AMP. REF.	MAGNITUDE
1	1	(RAMP)	0.	1	11	(RAMP)	0.
21	11	(RAMP)	1.00000E-06				

- (RAMP) OR (STEP) - INDICATE USE OF DEFAULT AMPLITUDES ASSOCIATED WITH THE STEP

FOR USE AT UNIVERSITY OF NOTRE DAME UNDER ACADEMIC LICENSE FROM HKS, INC.
STATIC DIFFUSION -- STRONGLY COUPLED Standard Case 1

W A V E F R O N T M I N I M I Z A T I O N

```
*WAVEFRONT MINIMIZATION, SUPPRESS
  WAVEFRONT MINIMIZATION HAS BEEN SUPPRESSED
```

P R O B L E M S I Z E

```
      NUMBER OF ELEMENTS IS                                  10
      NUMBER OF NODES IS                                     21
      NUMBER OF NODES DEFINED BY THE USER                    21
      NUMBER OF INTERNAL NODES GENERATED BY THE PROGRAM       0
      TOTAL NUMBER OF VARIABLES IN THE MODEL                 32
      (DEGREES OF FREEDOM PLUS ANY LAGRANGE MULTIPLIER VARIABLES)
      MAXIMUM D.O.F. WAVEFRONT ESTIMATED AS                   5
      RMS WAVEFRONT ESTIMATED AS                              5
      UNSYMMETRIC MATRIX STORAGE AND SOLUTION WILL BE USED
      FILE SIZES - THESE VALUES ARE IN WORDS AND ARE CONSERVATIVE UPPER BOUNDS
        UNIT          LENGTH
          21             500
          22             500
      IF THE RESTART FILE IS WRITTEN ITS LENGTH WILL BE APPROXIMATELY
                    1302 WORDS WRITTEN IN THE PRE PROGRAM
           PLUS      176 WORDS WRITTEN AT THE BEGINNING OF EACH STEP
           PLUS     1113 WORDS FOR EACH INCREMENT WRITTEN TO THE RESTART FILE
      ALLOCATED WORKSPACE                                     7013
                        END OF USER INPUT PROCESSING
  JOB TIME SUMMARY
    USER TIME   =   1.1167
    SYSTEM TIME =  0.21667
    TOTAL TIME  =   1.3333
```

S T E P 1 C O U P L E D - T E M P E R A T U R E - D I S P L A C E M E N T A N A L Y S I S

STEADY STATE ANALYSIS

AUTOMATIC TIME CONTROL WITH -
A SUGGESTED INITIAL TIME INCREMENT OF 5.000E-03
AND A TOTAL TIME PERIOD OF 1.00
THE MINIMUM TIME INCREMENT ALLOWED IS 1.000E-05
THE MAXIMUM TIME INCREMENT ALLOWED IS 5.000E-02
CREEP AND SWELLING EFFECTS ARE OMITTED IN THIS STEP

INCREMENT 25 SUMMARY

TIME INCREMENT COMPLETED 4.109E-02, FRACTION OF STEP COMPLETED 1.00
STEP TIME COMPLETED 1.00 , TOTAL TIME COMPLETED 1.00

E L E M E N T O U T P U T

THE FOLLOWING TABLE IS PRINTED FOR ALL ELEMENTS WITH TYPE U1 AT THE INTEGRATION POINTS

ELEMENT	PT	FOOT-NOTE	SDV1	SDV2	SDV3	SDV4	SDV5	SDV6	SDV7	SDV8	SDV9
1	1		6.4702E-06	2.4147E-05	4.1164E-07	3.9302E-07	4.1801E-07	3.8557E-07	-9.7924E-15	2.1133E-03	7.8868E-03
2	1		3.7114E-05	5.4863E-05	4.0606E-07	5.1782E-07	3.6322E-07	5.6252E-07	-9.7907E-15	1.2113E-02	1.7887E-02
3	1		6.7883E-05	8.5706E-05	6.9290E-07	1.0952E-06	5.4762E-07	1.2368E-06	-9.7890E-15	2.2113E-02	2.7887E-02
4	1		9.8780E-05	1.1668E-04	1.5199E-06	2.2277E-06	1.2666E-06	2.4959E-06	-9.7872E-15	3.2114E-02	3.7887E-02
5	1		1.2981E-04	1.4778E-04	2.8461E-06	3.8147E-06	2.4959E-06	4.1872E-06	-9.7854E-15	4.2114E-02	4.7888E-02

STEP 1 INCREMENT 25
TIME COMPLETED IN THIS STEP 1.00

ELEMENT	PT	FOOT-NOTE	SDV1	SDV2	SDV3	SDV4	SDV5	SDV6	SDV7	SDV8	SDV9
6	1		1.6096E-04	1.7901E-04	4.5449E-06	5.6773E-06	4.1574E-06	6.0946E-06	-9.7836E-15	5.2115E-02	5.7888E-02
7	1		1.9225E-04	2.1037E-04	6.3777E-06	7.1228E-06	6.1095E-06	7.4059E-06	-9.7817E-15	6.2115E-02	6.7889E-02
8	1		2.2367E-04	2.4187E-04	7.4208E-06	7.5549E-06	7.3910E-06	7.5996E-06	-9.7798E-15	7.2116E-02	7.7890E-02
9	1		2.5523E-04	2.7351E-04	7.1675E-06	6.0499E-06	7.5996E-06	5.6326E-06	-9.7778E-15	8.2117E-02	8.7891E-02
10	1		2.8692E-04	3.0528E-04	4.4703E-06	1.2815E-06	5.6028E-06	1.1921E-07	-9.7757E-15	9.2118E-02	9.7892E-02

N O D E O U T P U T

THE FOLLOWING TABLE IS PRINTED FOR ALL NODES

NODE	FOOT-NOTE	COOR1	U1	NT11
1		0.	0.	0.
2		5.0000E-03	1.2757E-08	
3		1.0000E-02	5.1029E-08	9.8132E-08
4		1.5000E-02	1.1487E-07	
5		2.0000E-02	2.0433E-07	1.9667E-07
6		2.5000E-02	3.1946E-07	
7		3.0000E-02	4.6031E-07	2.9561E-07
8		3.5000E-02	6.2695E-07	
9		4.0000E-02	8.1942E-07	3.9496E-07
10		4.5000E-02	1.0378E-06	
11		5.0000E-02	1.2821E-06	4.9473E-07
12		5.5000E-02	1.5524E-06	
13		6.0000E-02	1.8487E-06	5.9492E-07
14		6.5000E-02	2.1712E-06	
15		7.0000E-02	2.5198E-06	6.9553E-07
16		7.5000E-02	2.8946E-06	
17		8.0000E-02	3.2958E-06	7.9658E-07
18		8.5000E-02	3.7232E-06	
19		9.0000E-02	4.1771E-06	8.9807E-07
20		9.5000E-02	4.6574E-06	
21		0.1000	5.1642E-06	1.0000E-06

THE ANALYSIS HAS BEEN COMPLETED

STEP 1 INCREMENT 26
TIME COMPLETED IN THIS STEP 1.00

ANALYSIS COMPLETE

JOB TIME SUMMARY
USER TIME = 2.1167
SYSTEM TIME = 0.26667
TOTAL TIME = 2.3833

To appear in *Proceedings of the 5th International Conference on Hydrogen Effects on Material Behavior*, Jackson Lake Lodge, Wyoming, Sept. 1994.

MODELING OF HYDROGEN TRANSPORT IN CRACKING METAL SYSTEMS

J. P. Thomas and C. E. Chopin
University of Notre Dame
Department of Aerospace and Mechanical Engineering
374 Fitzpatrick Hall
Notre Dame, IN 46556-5637

Abstract

An extended stress-assisted diffusion theory with concentration induced deformations and equilibrium trapping effects was developed for modeling hydrogen transport in cracking metal systems. Special Fortran "user element" subroutines were written for the ABAQUS finite element code to solve the transport equations in 1-D geometries. A simple rod problem with a square-root singular stress was analyzed to assess the influence of the hydrogen induced deformation on the concentration and deformation field variables. Significant differences between the classical and extended stress-assisted diffusion theory were demonstrated and the implications for modeling crack tip hydrogen distributions discussed.

Introduction

Two fundamental questions naturally arise in modeling the influence of hydrogen on the crack growth rate of metals. Namely, how does hydrogen "enhance" the crack growth rate (CGR); and what is the relationship between the hydrogen distribution within the material and the corresponding "enhancement" in the CGR? Quantitative knowledge of the crack tip hydrogen distribution under service or laboratory test conditions is requisite to addressing these questions and will require: **a)** a hydrogen transport model that incorporates trapping and deformation-concentration coupling effects (governing equations); **b)** knowledge of the time dependent, non-uniform hydrogen distribution along the crack walls (boundary conditions); and **c)** a mathematical solution technique for the resulting system of non-linear equations.

Stress-assisted diffusion (SAD) theory [1] is commonly used to model hydrogen transport in cracking metals systems. This theory represents an extension of classical diffusion with a hydrostatic stress gradient term added as a driving force for diffusive transport. Equilibrium trapping effects are included through the use of an effective diffusion coefficient. The influence of hydrogen on the material deformation state is assumed to be negligible, and this uncouples the deformation equations from the concentration variable. Hydrostatic stresses determined from solutions to standard elasticity or plasticity problems are used with the SAD equation to solve for the resulting concentration. The steady-state hydrogen distribution for Mode I cracks in linear elastic materials with uniform hydrogen concentration along the boundaries is given by [2]:

$$c = c_0 \exp\left(constant \times \frac{K}{\sqrt{r}} \cos\frac{\theta}{2} \right)$$

where c_0 is the boundary concentration, K is the stress intensity factor, and r and θ are polar coordinates centered at the crack tip. An infinite hydrogen concentration is predicted at the crack tip. Transient and steady-state hydrogen distributions for a plastically deforming crack in iron have been obtained by Sofronis & McMeeking [3] using finite element methods. Their results show large, but finite, concentrations at the crack tip region, primarily in traps near the crack surface. They conclude that the crack tip hydrogen distribution is primarily determined by the creation of dislocation traps via plastic straining at the crack tip.

Damage models that attempt to link the crack tip hydrogen distribution to the fracture process have been reviewed in [4-6]. Applications to service cracking problems have met with some success, but the lack of information on the crack wall hydrogen distributions under service or laboratory conditions has limited the usefulness of these models.

The task of specifying the crack wall hydrogen distribution is difficult because of the complex nature of the interacting chemical, mechanical, and metallurgical processes operative during hydrogen assisted cracking of metals (Figure 1). In aqueous systems, the hydrogen production process is driven by the rapid and irreversible evolution of the chemically unstable "bare" surface at the crack tip to a more stable equilibrium "filmed" state. An electron flow is induced between the bare and filmed crack flank surfaces; net anodic (dissolution/filming) reactions take place on the bare surface and net cathodic (hydrogen reduction) reactions take place on the filmed surfaces.

Adsorbed hydrogen, H_{ads}, can be produced on both the bare and filmed crack surfaces by: **(1)** the reduction of hydrogen ions in acidic environments; or **(2)** by the reduction of water in alkaline environments. The MH_{ads} species are then free to be absorbed by the transition reaction **(a)**; or combine to form H_2 gas via: recombination **(b1)**; or electrochemical desorption **(b2)**. Reactions **(a)**, **(b1)**, and **(b2)** occur in parallel, but one of the two **(b1)** or **(b2)** reactions is usually dominant (Figure 2).

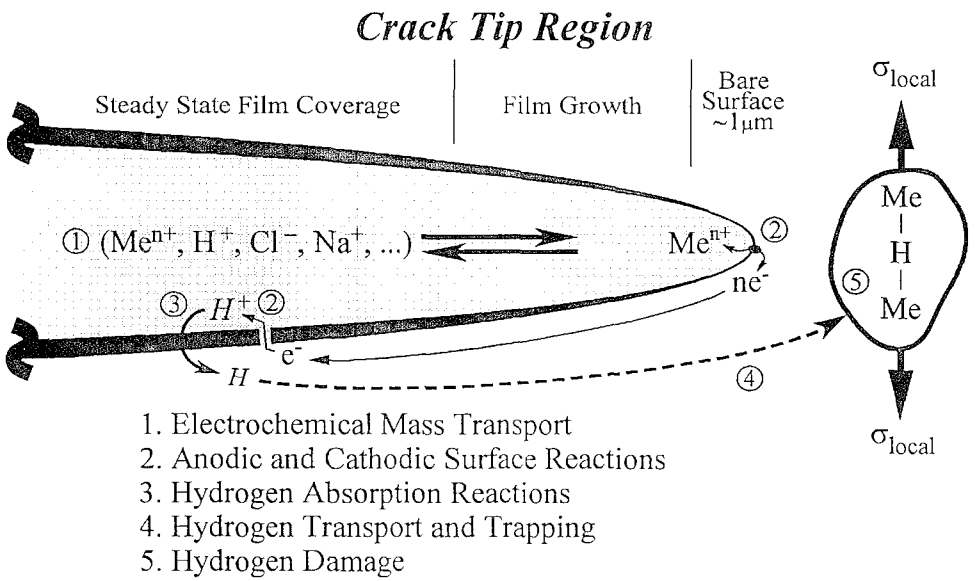


Figure 1: Schematic of the processes responsible for hydrogen assisted crack growth.

(1) ***Acidic:***	$M + H^+ + e^- \Leftrightarrow MH_{ads}$
(2) ***Alkaline:***	$M + H_2O + e^- \Leftrightarrow MH_{ads} + OH^-$

(a) ***Adsorption-Absorption:***	$MH_{ads} \Leftrightarrow MH_{abs}$
(b1) ***Recombination:***	$MH_{ads} + MH_{ads} \Leftrightarrow H_2 + 2M$
(b2) ***EC Desorption:***	$MH_{ads} + H^+ + e^- \Leftrightarrow H_2 + M$

Figure 2: Summary of the hydrogen producing reactions.

The distribution of MH_{abs} along the crack surface is governed by the surface coverage of MH_{ads} and the kinetics of reaction **(a)** acting in parallel with reaction **(b1)** or **(b2)**. These factors are influenced, in turn, by: the electrochemical environment at the crack tip region (e.g., the potential, pH, species concentrations, dissolved O_2, etc.); the kinetics of the bare and filmed surface reactions; and the rate of transport of H_{abs} from the crack surface into the material.

Iyer and Pickering [7] review and model the mechanisms and kinetics of hydrogen evolution and entry in stress free metallic systems with homogeneous electrochemical conditions at the metal surface. Their model is used to quantify the rate constants associated with reactions **(1)** or **(2)** and **(a)** and **(b1)** or **(b2)** via analysis of experimental permeation data. Turnbull [8] has reviewed electrochemical conditions in cracks with particular emphasis on corrosion fatigue cracks of structural steels in sea water. Similarly, Beck [9] and Newman [10] have examined experimental techniques for characterizing bare (and filmed) surface reaction kinetics. It seems that the above models, data, and techniques, plus information concerning the rate controlling process during crack growth, will have to be used in an analysis of the mass transport process within the crack to develop realistic predictions of the MH_{ads} distribution.

The objective of this paper is to address the above items **a)** and **c)**. A hydrogen transport model for isothermal linear elastic materials with mutual deformation-concentration coupling and equilibrium trapping is developed using continuum mixture theory. Computational solutions for 1-D geometries and arbitrary boundary conditions are obtained using the finite element code ABAQUS[1] supplemented with Fortran "user element" subroutines. The code is used to analyze hydrogen transport in a 4340 steel rod subjected to a singular body force($\sim A/x^{3/2}$) which produces a square root singular stress. The concentrations, displacements, and dilatational strains predicted by the fully coupled theory are somewhat larger than those predicted by classical SAD theory, depending on the extent of trapping. Further examination of the fully coupled theory in the context of hydrogen transport in 2-D crack systems is currently underway.

The paper begins with a description of the strongly coupled hydrogen transport model. The use of ABAQUS with its "user element" subroutines for solving 1-D problems is described next, followed by an analysis and discussion of hydrogen transport in a rod with a singular body force. Extension of the finite element model to 2-D geometries and its application to cracking metal systems is briefly discussed, followed by suggestions for future work.

[1] ABAQUS is a commercial finite element code supported by Hibbitt, Karlsson & Sorensen, Inc., Pawtucket, RI.

Modeling the Hydrogen Transport and Trapping Process

Three species of hydrogen are modeled in the analysis:

$H_L \equiv$ interstitial or lattice hydrogen

$H_R \equiv$ weak or moderately (reversibly) trapped hydrogen (e.g., $\Delta E_b \leq 30$)

$H_I \equiv$ strongly (irreversibly) trapped hydrogen (e.g., $\Delta E_b > 30$ kJ/mol)

Balance Equations

Balance equations for the mixture mass, the three hydrogen species masses, the mixture linear momentum and moment of momentum, mixture energy, and mixture entropy can be written. Since our modeling considerations are restricted to isothermal linear elastic materials, only the balance equations for the hydrogen species mass and the mixture linear momentum (assuming negligible inertial effects) need be explicitly considered. They are given by:

Mass :
$$\frac{\partial c_k}{\partial t} + \vec{\nabla} \cdot \vec{\mathcal{J}}_k = a_k \qquad (k = L,\ R,\ or\ I) \tag{1}$$

Linear Momentum:
$$\sigma_{ij,j} + F_i = 0 \qquad (i, j = x,\ y,\ or\ z) \tag{2}$$

where: $c_k \equiv$ mass fraction concentrations for H_k $[kg/kg]$.
$\vec{\mathcal{J}}_k \equiv$ concentration flux vectors for H_k $[kg/kg \cdot m/s\,]$.
$a_k \equiv$ mass supply rates for H_k $\left[kg/kg/s\right]$.
$\sigma_{ij} \equiv$ stress tensor $\left[N/m^2\right]$.
$F_i \equiv$ the i^{th} component of body force vector $\left[N/m^3\right]$.

Trapping Analysis

Expressions for the mass supply rates a_k in Eq. (1) are written in accordance with the trapping model of McNabb & Foster [11]:

Stoichiometry:
$$H_L \Leftrightarrow H_R \quad \text{and} \quad H_L \Rightarrow H_I \tag{3}$$

The stoichiometric relations require the supply terms sum to zero (i.e., $a_R + a_I = -a_L$).

Kinetics of Trapping:
$$a_R = k_R^f(1-\theta_{_R})c_L - k_R^b\theta_{_R} \tag{4}$$
$$a_I = k_I^f(1-\theta_{_I})c_L - k_I^b\theta_{_I} \approx k_I^f(1-\theta_{_I})c_L$$

where: $k_R^f,\ k_I^f,\ k_R^b,\ k_I^b \equiv$ forward and backward trap rate constants for H_R and H_I $[1/s]$.
$\theta_{_R}$ and $\theta_{_I} \equiv c_R/c_R^s$ and c_I/c_I^s, respectively, are the fraction of filled trap sites [1].
c_R^s and $c_I^s \equiv$ saturation mass fraction concentration of H_R and H_I $[kg/kg]$.

The quantities $k_R^f,\ k_I^f,\ k_R^b,\ k_I^b,\ c_R^s$ and c_I^s are related to trap site densities, probability of capture, etc. and can be determined from experimental measurements (e.g., [12-14]).

Significant simplifications are effected when the rate constants for trapping are much greater than those for diffusive transport. Trapping can then be modeled as a steady-state process (i.e., $a_L = a_R = a_I = 0$). This case is considered below.

SS Trapping:

$$c_R = \frac{c_R^s\, K_R\, c_L}{1 + K_R\, c_L} \approx c_R^s\, K_R\, c_L \quad \& \quad c_I = c_I^s \tag{5}$$

$$K_R \equiv \frac{k_R^f}{k_R^b} = \exp\left(\frac{-\Delta E_b}{\mathbb{R}\,T}\right)$$

so that the total internal hydrogen concentration is simply a linear function of $c_L(x_i, t)$:

$$c_{TOTAL}(x_i, t) = c_L(x_i, t) + c_R(x_i, t) + c_I(x_i, t) = (1 + c_R^s\, K_R) c_L(x_i, t) + c_I^s \tag{6}$$

The three versions of Eq. (1) can be summed to give a single equation by the following considerations. First, $\vec{\mathcal{J}}_R = \vec{\mathcal{J}}_I = 0$ because of the linear elastic material assumption which precludes trap site motion (e.g., dislocation motion during plastic deformation). And second, from Eq. (5a):

$$\frac{\partial c_R}{\partial t} \approx c_R^s\, K_R\, \frac{\partial c_L}{\partial t} \quad \text{and} \quad \frac{\partial c_I}{\partial t} = 0 \tag{7}$$

The resulting mass balance equation is given by:

$$(1 + c_R^s\, K_R)\frac{\partial c_L}{\partial t} + \vec{\nabla} \cdot \vec{\mathcal{J}}_L = 0 \tag{8}$$

Constitutive Equations

Mass Flux:

$$\vec{\mathcal{J}}_L = -\frac{c_L\, D_L}{R_L\, T} \vec{\nabla} \mu_L \quad \textit{Linear Onsager Relation} \tag{9}$$

where μ_L is the *mass* based chemical potential [15] defined by:

$$\mu_L \equiv \frac{\partial \psi}{\partial c_L} = \frac{1}{\mathcal{M}_L}\left(\mu_L^o(T) + \mathbb{R}T \ln(c_L) - \overline{V}_H k e\right) \quad \left[\frac{J}{g}\right] \tag{10}$$

and:

$D_L \equiv$ diffusion coefficient for H_L $[m^2/s]$.

$R_L \equiv$ gas constant for $H_L = \mathbb{R}/\mathcal{M}_L$ $[J/kg \cdot {}^\circ K]$.

$\mathcal{M}_L \equiv$ molecular mass of hydrogen $[kg/mol]$.

$T \equiv$ temperature $[^\circ K]$.

$\psi \equiv \psi(c_L,\, c_R,\, c_I; \epsilon_{ij}\,;\, T)$ free energy per unit mixture mass $[J/kg]$.

$\mu_L^o(T) \equiv$ reference potential for H_L at temperature T $[J/kg]$.

$\overline{V}_H \equiv$ partial molar volume of hydrogen in the metal $[m^3/mol\, H]$.

$k \equiv$ bulk modulus of elasticity $[N/m^2]$.

$e \equiv$ trace of the strain tensor (i.e., $e = \epsilon_{ii} = \epsilon_{11} + \epsilon_{22} + \epsilon_{33}$) $[m/m]$.

The use of mass based chemical potentials simplifies the analysis of fully coupled deformation-diffusion processes because of the primary role played by mass in the deformation equations.

The resulting expression for concentration flux is given by:

$$\vec{\mathcal{J}}_L = -D_L\, \vec{\nabla} c_L + \frac{\overline{V}_H\, D_L}{\mathbb{R}\, T}\, k c_L \vec{\nabla} e \tag{11}$$

The constitutive equation for the stress consists of Hooke's law combined with a dilatational stress contribution due to changes in the total hydrogen concentration:

Stress: $$\sigma_{ij} \equiv \rho \frac{\partial \psi}{\partial \epsilon_{ij}} = \lambda\, e\, \delta_{ij} + 2G\epsilon_{ij} - 3\, k\, \alpha_H\, (1 + c_R^s K_R)\Delta\, c_L\, \delta_{ij} \tag{12}$$

where $\rho \equiv$ mass density of the solid $[kg/m^3]$.
$\lambda \equiv$ Lame´ constant $[N/m^2]$.
$\delta_{ij} \equiv$ Kronecker delta ($\delta_{ij} = 1$ for $i = j$ and 0 otherwise).
$G \equiv$ shear modulus $[N/m^2]$.
$\epsilon_{ij} \equiv \frac{1}{2}\,(u_{i,j} + u_{j,i})$ infinitesimal strain tensor $[m/m]$.
$u_i \equiv$ the i^{th} component of the displacement vector $[m]$.
$\alpha_H \equiv$ linear expansion coefficient for internal hydrogen $= \frac{1}{3}\frac{\rho}{\mathcal{M}_L}\overline{V}_H$ $[m/m/\Delta c_H]$.
$(1 + c_R^s K_R)\Delta c_L \equiv$ change in c_{total} from some reference level.

The relationship between the chemical potential and stress (Eqs. (10) and (12)) is dictated by the thermodynamic reciprocity relationship:

$$\frac{\partial \mu_L}{\partial \epsilon_{ij}} = \frac{\partial(\sigma_{ij}/\rho)}{\partial c_L} \tag{13}$$

Governing Equations

Combining the mass and momentum balance equations with the constitutive relations results in the following system of governing equations for transport:

Diffusion Equation:

$$\frac{\partial c_L}{\partial t} = D_{eff}\, \nabla^2 c_L - \frac{\overline{V}_H\, D_{eff}}{\mathbb{R}\, T} k\Big(\, \vec{\nabla} c_L \cdot \vec{\nabla} e + c_L \nabla^2 e\Big) \tag{14}$$

Deformation Equations ($i = 1,\ 2,\ 3$):

$$(\lambda + G)\, \frac{\partial e}{\partial x_i} + G\, \nabla^2 u_i + F_i = 3k\, \alpha_H (1 + c_R^s\, K_R) \frac{\partial c_L}{\partial x_i} \tag{15}$$

where D_{eff} is an "effective" diffusion coefficient defined by: $D_{eff} \equiv D_L/(1 + c_R^s K_R)$.

Equation (14) is identical to the stress-assisted diffusion equations published in the literature with the exception of the $\nabla^2 e$ term which is identically zero when linear elastic material behavior is assumed (and $F_i = 0$). In the present formulation it is given by:

$$\nabla^2 e = \frac{3k\, \alpha_H}{\lambda + 2G} (1 + c_R^s\, K_R) \nabla^2 c_L \tag{16}$$

Computational Modeling

Equations (14) and (15) form a system of non-linearly coupled partial differential equations that must be solved for c_L and u_i as functions of the space and time coordinates (x_i, t). This is accomplished for 1-D geometries by writing Fortran "user element" subroutines for the ABAQUS finite element code to effect a computational solution. The 1-D "plane stress" form of the governing equations[2] ($\sigma_{yy} = \sigma_{zz} = 0$) is given by

[2] "Plane strain" forms of the 1-D equations can be obtained by a simple change in constants.

Diffusion:

$$(1 + c_R^s K_R)\frac{\partial c_L}{\partial t} + \frac{\partial \mathcal{J}_L}{\partial x} = 0 \tag{17}$$

$$\mathcal{J}_L = -D_L\frac{\partial c_L}{\partial x} + \frac{\overline{V}_H D_L}{\mathbb{R}T} k c_L \frac{\partial e}{\partial x}$$

Deformation:

$$\frac{\partial \sigma_x}{\partial x} + F_x = 0 \tag{18}$$

$$\sigma_x = 3k(e - 3\alpha_H (1 + c_R^s K_R)\Delta c_L) = E\left(\frac{\partial u}{\partial x} - \alpha_H (1 + c_R^s K_R)\Delta c_L\right)$$

A single differential equation for c_L can be obtained by combining Eqs. (17) and (18):

$$\frac{\partial c_L}{\partial t} = \frac{\partial}{\partial x}\left[D_{eff}\left(1 - \frac{\rho \overline{V}_H^2 k}{\mathcal{M}_L \mathbb{R}T}(1 + c_R^s K_R)c_L\right)\frac{\partial c_L}{\partial x} + \frac{\overline{V}_H D_{eff}}{3\mathbb{R}T}F_x c_L\right] \tag{19}$$

which, in the absence of body forces, is a standard diffusion equation with a concentration dependent diffusion coefficient. Solutions to the steady-state problem, with and without body forces, can be obtained by integration (symbolic computation is highly recommended).

A coupled set of equations for a single finite element of length h and cross-sectional area A can be written from Eqs. (17-18) using the method of weighted residuals. The result, after integration by parts, is given by:

$$\int_0^h \left((1 + c_R^s K_R)\frac{\partial c_L}{\partial t}\{G_i(x)\} - \mathcal{J}_L\left\{\frac{\partial G_i(x)}{\partial x}\right\}\right) dx = -\mathcal{J}_L\{G_i(x)\}\Big|_0^h \tag{20}$$

$$\int_0^h \left(-\sigma_x\left\{\frac{\partial H_j(x)}{\partial x}\right\} + F_x\{H_j(x)\}\right) dx = -\sigma_x\{H_j(x)\}\Big|_0^h$$

where:

$$c_L \equiv \sum_{i=1}^{2} G_i(x)c_i(t) = \lfloor G_i(x)\rfloor\{c_i(t)\} \qquad i = 1, 2 \tag{21}$$

$$u \equiv \sum_{j=1}^{3} H_j(x)u_j = \lfloor H_j(x)\rfloor\{u_j\} \qquad j = 1, 2, 3$$

are 2 and 3 node finite element representations for the lattice concentration and displacement, $G_i(x)$ and $H_j(x)$ are the respective linear and quadratic interpolation functions, and $\lfloor\cdots\rfloor$ indicates a row matrix while $\{\cdots\}$ indicates a column matrix.

Substituting Eqs. (21) into (17b) and (18b) and converting to isoparametric coordinates, results in finite element equations of the form:

$$\begin{bmatrix} [C_c] & [0] \\ [0] & [0] \end{bmatrix}\begin{Bmatrix} \{\dot{c}_i\} \\ \{\dot{u}_j\} \end{Bmatrix} + \begin{bmatrix} [K_c] & [K_{cu}] \\ [K_{uc}] & [K_u] \end{bmatrix}\begin{Bmatrix} \{c_i\} \\ \{u_j\} \end{Bmatrix} = \begin{Bmatrix} \{R_c\} \\ \{R_u\} \end{Bmatrix} \tag{22}$$

The capacitance, stiffness, and RHS matrices, $[C]$, $[K]$, and $\{R\}$, are functions of c_L and u, which necessitates the use of nonlinear solution techniques. The integrations required for the computation of the $[C]$ and $[K]$ matrices are accomplished using two-point Gauss quadrature.

The term $\partial e/\partial x$ in $\mathcal{J}_L$ includes the second derivative in u (from Eq. (18b):

$$\frac{\partial e}{\partial x} = (1-2\nu)\frac{\partial^2 u}{\partial x^2} + 2(1+\nu)\alpha_H\,(1 + c_R^s K_R)\frac{\partial c_L}{\partial x} \tag{23}$$

This would normally require the use of C^1 continuous elements in order for u to satisfy the element interface compatibility requirement [16]. To avoid this complication, we use the values of u and c_L from the previous time step to approximate $\partial e/\partial x$ in the current time calculations.

The deformation equations are analogous to those of linear thermoelasticity. This allows the use of ABAQUS' coupled temperature-displacement routine to solve the problem. Time integration is performed using an implicit backwards difference scheme. The computations and setup required of the user element subroutine include [17]: calculation of the $[C]$, $[K]$ and $\{\mathrm{R}\}$ matrices; calculation of the "Jacobian" and {right-hand-side} matrices for the Newton-Raphson non-linear solver routine; and updating the solution dependent state variables: $\mathcal{J}_L, \sigma_x$, e, and $\partial e/\partial x$. The subroutine is written in double precision Fortran, and the code is run on a Sun SPARC10 workstation.

Applications

Steady-state hydrogen transport in a 4340 steel rod subjected to a body force selected to give a $1/\sqrt{x}$ singular stress (Figure 3) was studied using the ABAQUS code. The rod was discretized using 200 elements of length $l_i = 0.104/0.94^{i-1}\,[\mu m]$, where the first and smallest element ($l_1 = 0.104\,[\mu m]$) was placed at the left-hand end of the bar ($x = 4 \times 10^{-3}\,[cm]$). The parameter values used in the analysis were: $\rho = 7.8\,[g/cm^3]$; T=293 [K]; $D_L = 1 \times 10^{-5}$ $[cm^2/s]$; $\overline{V}_H = 2.0\,[cm^3/mol]$; $\mathcal{M}_L = 1.008\,[g/mol]$; $(1 + c_R^s K_R) = 20$ (low trapping) & 500 (high trapping); $E = 200\,[GPa]$; $\nu = 0.3$; $F_x = 15 \times 10^6\,[N/m^3]$, and $(c_L)_{ref} = 0$.

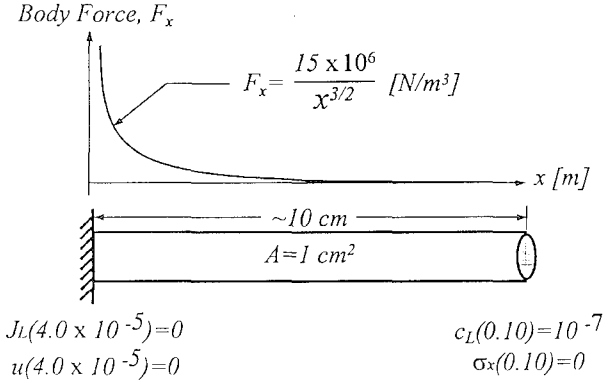


Figure 3: The rod geometry with the applied body force and boundary conditions.

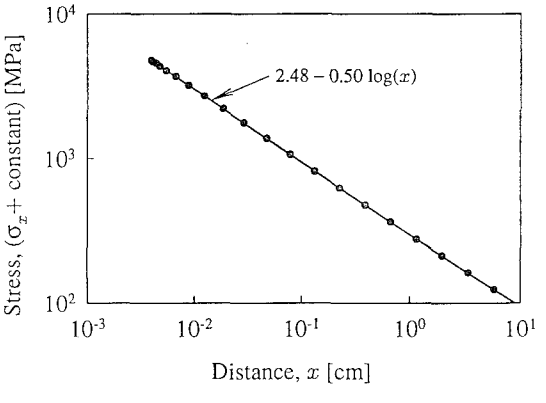


Figure 4: Gauss integration point stresses with a least squares line fit through the data.

Results

An analytical solution to this problem[3] was obtained by direct integration of Eq. (19). The singular nature of the body force results in a mathematical solution for the concentration that is a multi-valued function of x. In order to avoid the multiple concentration values, we must restrict

[3] To be described in more detail in a future publication.

our considerations to the region $x > 4 \times 10^{-3}\,[cm]$. The difficulty arises when the sign of the $\partial c_L/\partial x$ coefficient term in Eq. (19) changes from positive to negative. That is, when c_L exceeds some "critical" value given by: $\mathcal{M}_L\,\mathbb{R}\,T/\rho\,\overline{V}_H^2\,k(1+c_R^s\,K_R)$.

Figures 4 through 8 show the steady-state analytical and finite element (FE) results (every $20th$ point) for the high and low trapping conditions. Figure 4 shows the FE stresses at the Gauss integration points with a least squares fit line through the FE data. The stress in this problem is not influenced by the hydrogen; it is simply related to the integral of the body force per Eq. (18a). The required square root singularity in the stress is clearly predicted by the FE code as indicated by the slope of the least squares line fit.

Figures 5 & 6 show the concentration distribution for the fully coupled and stress-assisted diffusion (SAD) theories with $\sigma_{HYD} = 10 \times 10^6/\sqrt{x}$. The fully coupled model predicts larger concentrations than the SAD model as the singularity is approached, and the difference increases as the degree of trapping increases (i.e., $1 + c_R^s K_R = 500$ -vs.- 20). Figure 6 shows that the fully coupled concentration singularity is more severe than the exponential square root singularity of the SAD model for the higher trapping case.

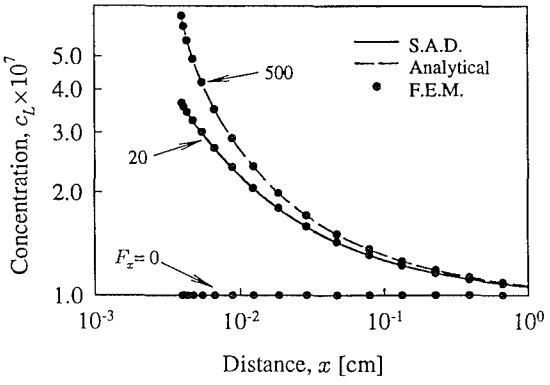


Figure 5: Concentration predictions for the fully coupled and SAD theory under high and low trapping conditions.

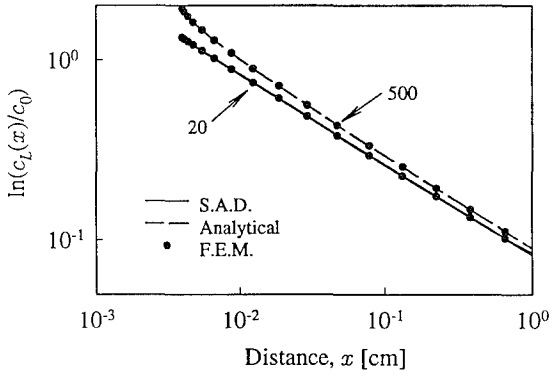


Figure 6: Plot to illustrate the difference in singular behavior between the fully coupled and SAD model concentration predictions.

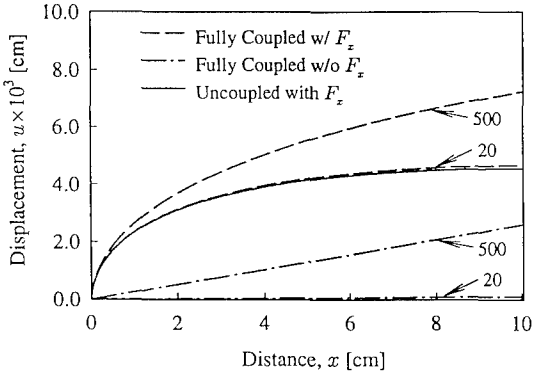


Figure 7: Nodal displacement curves for a variety of conditions.

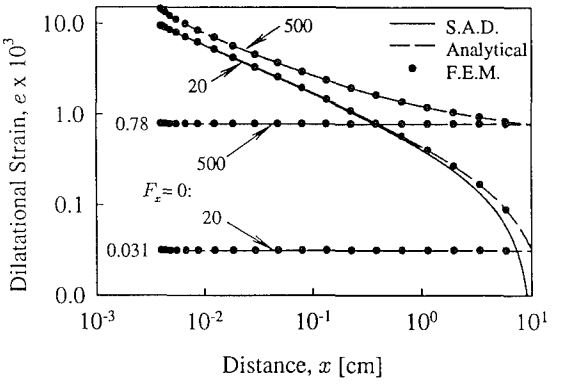


Figure 8: Analytical and FE dilatational strains for a variety of conditions.

Figures 7 & 8 show nodal displacement curves and Gauss point dilatational strains, respectively. The fully coupled theory predicts larger displacements and dilatational strains throughout the rod. Again, the differences increase as the degree of trapping increases. The displacements and strains for the zero body force case are also shown.

Discussion

This simple rod problem with its square root singular stress clearly illustrates the differences between the fully coupled and classical SAD models. The concentration differences are relatively small but dependent on the trapping constants (i.e., the amount of trapped hydrogen). The non-physical nature of the multi-valued concentration in the fully coupled theory may be an indication that singularities, like the inverse square root singularity found at 2-D crack tips in classical elasticity, do not naturally arise in the fully coupled theory. This could have important implications in modeling the hydrogen damage at 2-D crack tips.

The influence of the concentration coupling to the deformation state, and its role in the hydrogen damage process, is also an important consideration. The fully coupled theory exhibits larger dilatational strains than those predicted by SAD theory (classical elasticity), but identical stresses. On the other hand, a bar fixed between two walls and subject to a change in concentration results in differences between both strain *and* stress. This is also likely to be true in two and three-dimensional problems where the deformations in different directions are coupled through the constitutive equations.

The results suggest the need for an examination of the coupled theory in the context of crack tip hydrogen predictions. We are currently developing 2-D isoparametric rectilinear (8-node displacement; 4-node concentration) and axisymmetric user element routines for use in this task. Extension of the model to include the effects of non-equilibrium trapping, crack tip plasticity, and hydride formation will be considered in the future.

Acknowledgments

The discussions with Dr. D. Kirkner concerning the finite element aspects of this work, and the support of this work by the Office of Naval Research under Contract No. N00014-93-1-0845, are both gratefully acknowledged.

References

1. J. C. M. Li, R. A. Oriani, & L. S. Darken, *Z. Physik. Chem.*, 1966, Vol. 49, pp. 271-290.
2. H. W. Lui, *Trans. ASME-J. Basic Engng.*, 1970, Vol. 92, pp. 633-638.
3. P. Sofronis, and R. M. McMeeking, *J. Mech. Phys. Solids*, 1989, Vol. 37, pp. 317-350.
4. H. K. Birnbaum, in *Environment-Induced Cracking of Metals*, R. Gangloff and M. B. Ives, Eds., National Association of Corrosion Engineers, Houston, TX, 1990, pp. 21-29.
5. *Hydrogen Degradation of Ferrous Alloys*, R. A. Oriani, J. P. Hirth, and M. Smialowski, Eds., Noyes Publications, Park Ridge, NJ, 1985.
6. J. P. Hirth, *Metall. Trans. A*, 1980, Vol. 11A, pp. 861-890.
7. R. N. Iyer and H. W. Pickering, *Annu. Rev. Mater. Sci.*, 1990, Vol. 20, pp. 299-338.
8. A. Turnbull, *Reviews in Coatings and Corrosion*, 1982, Vol. 5, pp. 43-171.
9. Beck, T. R., (1977), in *Electrochemical Techniques in Corrosion*, R. Baboian, Nat. Assoc. of Corrosion Engineers, Houston, TX, 27-34.

10. Newman, R. C., (1984), in *Corrosion Chemistry Within Pits, Crevices, and Cracks*, A. Turnbull, Ed., Her Majesty's Stationery Office, London, UK, 317-356.
11. A. McNabb and P. K. Foster, *Trans. TMS-AIME*, 1963, Vol. 227, pp. 618-627.
12. B. G. Pound, *Acta Metall. Mater.*, 1991, Vol. 39, pp. 2099-2105.
13. H. H. Johnson, *Metall. Trans. A*, 1988, Vol. 19A, pp. 2371-2387.
14. R.Oriani, *Acta Metall.*, 1970, Vol. 18, pp. 147-157.
15. J. P. Thomas, *Int. J. Engng. Sci.*, 1993, Vol. 31, pp. 1279-1294.
16. K. H. Huebner and E. A. Thorton, *The Finite Element Method for Engineers*, 2nd ed., J. Wiley & Sons, NY, 1982, pp. 79-85.
17. *ABAQUS Theory and User's Manuals,* Standard Version 5.3-1, Hibbitt, Karlson, & Sorensen, Inc., Pawtucket, RI, 1993.

APPENDIX F: Summary Of The Publications/Reports/Presentations

1. Papers Published in Refereed Journals:

1. J. P. Thomas and R. P. Wei, "Standard Error Estimates for Rates of Change From Indirect Measurements", *TECHNOMETRICS*, (in review).
2. J. P. Thomas and P. Matic, "Solute Transport Modeling in Elastic Solids", *International Journal of Engineering Science*, in preparation.

2. Non-Refereed Publications and Technical Reports:

1. J. P. Thomas and C. E. Chopin, "Modeling of Hydrogen Transport in Cracking Metal Systems", *Proceedings of the 5th International Conference on Hydrogen Effects on Material Behavior*, A. W. Thompson and N. R. Moody, Eds., The Materials Society (TMS), Jackson Lake Lodge, Wyoming, Sept. 1994 (to appear).
2. J. P. Thomas and C. E. Chopin, "An ABAQUS User Element Routine for One-Dimensional Coupled Deformation-Diffusion Problems", *Department of Aerospace and Mechanical Engineering Report*, University of Notre Dame, Department of Aerospace and Mechanical Engineering, Notre Dame, IN, (in preparation).

3. Presentations

a. Invited:

1. J. P. Thomas, April 1994, "Modeling the Influence of Hydrogen on the Crack Growth Rate of Metals", Lehigh University, Department of Mechanical Engineering and Mechanics, Bethlehem, PA.
2. J. P. Thomas, July 1994, "Environmental Effects in Fatigue Crack Growth", Ladish Corporation, Inc., Cudahy, Wisconsin.
3. J. P. Thomas, October 1994, Invited Lecture, "Solute Transport in Elastic Solids", D. G. B. Edelen Symposium, 31st Annual Technical Meeting of the Society of Engineering Science (SES), College Station, Texas.
4. J. P. Thomas, October 1994, "Modeling the Influence of Internal Hydrogen on the Crack Growth Rate of Metals", University of Kentucky, Department of Engineering Mechanics, Lexington, Kentucky.
5. J. P. Thomas, January 1995, "Modeling the Influence of Internal Hydrogen on the Crack Growth Rate of Metals", Westinghouse Electric Corporation, Bettis Atomic Power Laboratory, West Mifflin, Pennsylvania.

b. Contributed:

1. J. P. Thomas, September 1994, "Modeling Crack Tip Hydrogen Distributions", Poster Session, 5th International Conference on *Hydrogen Effects on Material Behavior*, The Materials Society (TMS), Jackson Lake Lodge, Wyoming.
2. J. P. Thomas and C. E. Chopin, October 1994, "Finite Element Modeling of Hydrogen Transport in Metals", 31st Annual Technical Meeting of the Society of Engineering Science (SES), College Station, Texas (planned).

4. Books: none

5. List Of Honors/Awards:

Name of Person Receiving Award	Recipient's Institution	Name, Sponsor and Purpose of the Award
Mr. Charles E. Chopin, Graduate Student	Department of Aerospace and Mechanical Engineering University of Notre Dame Notre Dame, IN	SES 31st Annual Technical Meeting Student Stipend National Science Foundation & Office of Naval Research To support student participation in the SES Annual Meeting.

6. Participants And Their Status

Principal Investigator:
1. Dr. James P. Thomas, Assistant Professor, University of Notre Dame, Department of Aerospace and Mechanical Engineering, Notre Dame, IN.

Graduate Student:
1. Mr. Charles E. Chopin, 2nd year Doctoral Student, University of Notre Dame, Department of Aerospace and Mechanical Engineering, Notre Dame, IN.